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Published in:
Organic letters

DOI:
10.1021/ol402408v

Publication date:
2013

SUPPORTING INFORMATION

Catalytic Direct Cross-Coupling of Organolithium Compounds with Aryl chlorides

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Table of Contents

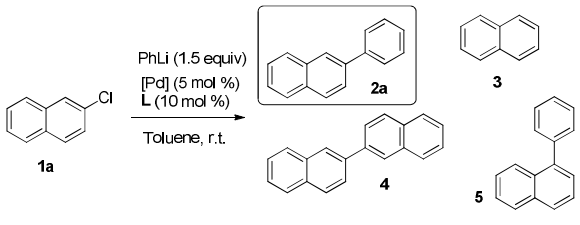
General methods:

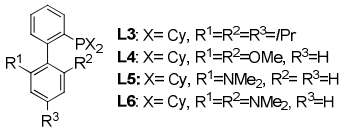
All reactions were carried out under a nitrogen atmosphere using oven dried glassware and using standard Schlenk techniques. THF and toluene were dried and distilled over sodium. $Pd_2(dba)_3$, SPhos, XPhos, DavePhos, CPhos, Qphos, P(^{t}Bu)$_3$, PCy$_3$ and Pd-PEPPSI-Ipent were purchased from Aldrich and used without further purification. ^{n}BuLi (1.6 M solution in hexane) and PhLi (1.8 M solution in dibutylether) were purchased from Acros. ThienylLi (1.0 M in THF/hexane), ^{tert}BuLi (1.7 M in pentane) and the compounds used as precursor for the preparation of lithium reagents, namely furan, 1-bromo-2,3-dimethyl-benzene, 1-bromo-2-methoxybenzene and 1-bromo-2-(methoxymethoxy)benzene were purchased from Aldrich. All the chlorides were commercially available and were purchased from TCI Europe N.V. with the exception of 1-chloro-4-methoxybenzene (Aldrich). Organolithium reagents other than the aforementioned were prepared according to described procedures (see below).

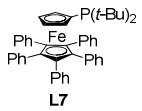
Chromatography: Merck silica gel type 9385 230-400 mesh, TLC: Merck silica gel 60, 0.25 mm. Components were visualized by UV and cerium/molybdenum or potassium permanganate staining. Progress and conversion of the reaction were determined by GC-MS (GC, HP6890: MS HP5973) with an HP1 or HP5 column (Agilent Technologies, Palo Alto, CA). Mass spectra were recorded on an AEI-MS-902 mass spectrometer (EI+) or a LTQ Orbitrap XL (ESI+). ^{1}H- and ^{13}C-NMR were recorded on a Varian AMX400 (400 and 100.59 MHz, respectively) using $CDCl_3$ as solvent. Chemical shift values are reported in ppm with the solvent resonance as the internal standard ($CHCl_3$: δ 7.26 for ^{1}H, δ 77.0 for ^{13}C). Data are reported as follows: chemical shifts, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constants (Hz), and integration. Carbon assignments are based on APT ^{13}C-NMR experiments.

Optimization Study: Additional Data

Table S1. Additional optimization data of the reaction between 1a and PhLi



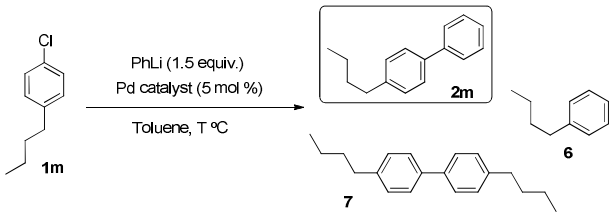




entry[a]	[Pd]	Ligand	Conv. (%)	**2a**:**3**:**4**:**5**[b]
1	**$Pd_2(dba)_3$**	**L4**,SPhos	55	51:0:0:4
2	**$Pd_2(dba)_3$**	**L5**,DavePhos	58	48:0:0:11
3	**$Pd_2(dba)_3$**	**L6**,CPhos	79	68:0:0:11
4	**$Pd_2(dba)_3$**	**L7**,QPhos	42	32:0:0:10

[a]Conditions: PhLi (0.45 mmol, 1.8 M solution in dibutyl ether diluted with THF to a final concentration of 0.6 M) was added to a solution of 2-chloronaphthalene (0,3 mmol) in toluene (2 mL unless otherwise noted). [b]**2a**:**3**:**4**:**5** ratios determined by GC analysis. [c]7.5 mol% was used. [d]In 1 mL of toluene. dba = dibenzylideneacetone.

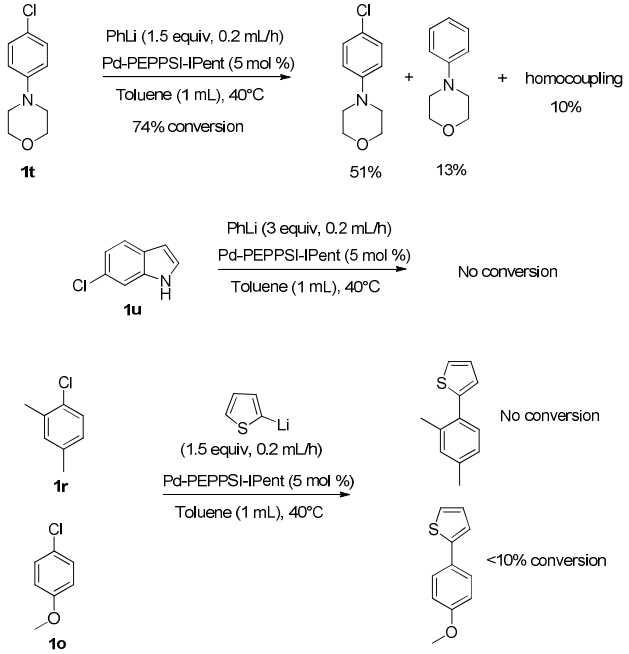
Table S2. Additional optimization data of the reaction between 1m and PhLi



entry[a]	[Pd]	TºC	PhLi flow-rate (mL/h)	Conv. (%)	**2m:6:7**[b]
1	**$Pd_2(dba)_3$/L3**	50	1	76	70:<1:6
2	**$Pd_2(dba)_3$/L3**	50	0.33	Full	88:<1:12
3	**$Pd_2(dba)_3$/L3**	35	0.33	64	61:<1:<3
4	**$Pd_2(dba)_3$/L3**	40	0.33	82	77:<1:5
5	**$Pd_2(dba)_3$/L3**	45	0.33	80	70:4:6
6[c]	**$Pd_2(dba)_3$/L3**	40	0.33	96	86:2:8
7[c,d]	**$Pd_2(dba)_3$/L3**	40	0.2	Full	89:3:8
8[c]	**Pd-PEPPSI-IPent**	40	0.2	Full	90:4:6
9[c]	**Pd-PEPPSI-IPent**	30	0.2	90	81:5:4

[a]Conditions: Phenyllithium (1.8 M solution in dibutyl ether diluted with THF to a final concentration of 0.6M) was added to a solution of 1-butyl-4-chlorobenzene (0.3 mmol) in toluene (2 mL unless otherwise noted). [b]**2m:6:7** ratios determined by GC-analysis. [c]In 1 mL of toluene. [d]Phenyllithium was diluted with toluene (instead of THF) to reach 0.6 M concentration. dba, dibenzylideneacetone.

Scheme S1. Pd-catalyzed cross-coupling of aryl lithium reagents with deactivated aryl chlorides: Scope Limitations



The Pd-catalyzed cross-coupling with aryl lithium reagents did not proceed efficiently when very deactivated aryl chlorides were used. The reaction between 4-(4-chlorophenyl)morpholine **1t** and PhLi led to low conversion and a mixture of products while the use of 6-chloroindole **1u** gave no reaction. Although it was used efficiently in the Pd-catalyzed cross-coupling with activated aryl chlorides, the less reactive thienyl lithium could not be coupled with deactivated and hindered aryl chlorides.

General procedures for the cross-coupling of aryl lithium reagents with aryl chlorides

Catalytic system A:

In a dry Schlenk flask Pd-PEPPSI-IPent (5 mol%, 0.015 mmol, 11.9 mg) and the substrate (0.3 mmol) were dissolved in 1 mL of dry toluene and the solution was stirred at the indicated temperature. The corresponding lithium reagent (1.5 equiv) was diluted with THF to reach the concentration of 0.6 M; this solution was slowly added with the indicated flow rate by the use of a syringe pump. After the addition was completed a saturated aqueous solution of NH_4Cl was added and the mixture was extracted with ether (3 x 5 mL). The organic phases were combined and dried with anhydrous Na_2SO_4. Evaporation of the solvent under reduced pressure afforded the crude product that was then purified by column chromatography.

Note: Thienyllithium (1.5 equiv) was diluted with toluene to reach a concentration of 0.6 M and TMEDA (1.5 equiv) was added. The resulting solution was slowly added with a flow rate of 0.5 mL/h to the reaction mixture warmed at 40 °C.

Catalytic system B:

In a dry Schlenk flask $Pd_2(dba)_3$ (2.5 mol%, 0.0075 mmol, 6.87 mg) and XPhos (10 mol%, 0.03 mmol, 14.3 mg) were dissolved in toluene, the substrate (0.3 mmol) was added and the solution stirred at the indicated temperature. The corresponding lithium reagent (1.5 equiv) was diluted with THF to reach a concentration of 0.6 M; this solution was slowly added with the indicated flow rate by the use of a syringe pump. After the addition was completed a saturated solution of aqueous NH_4Cl was added and the mixture was extracted with ether (3 x 5 mL). The organic phases were combined and dried with anhydrous Na_2SO_4. Evaporation of the solvent under reduced pressure afforded the crude product that was then purified by column chromatography.

Preparation of organolithium reagents:

A. 2,3-Dimethyl-phenyllithium and 2-Methoxy-phenyllithium

In a dry Schlenk flask the corresponding aryl bromide (1.8 mmol) was dissolved in dry THF (0.9 mL) and the solution was cooled down to -78 ºC. ^{t}BuLi (2 equiv) was added slowly and the solution was stirred for 1 h. Then the solution was allowed to reach room temperature.

B. Furyllithium[1]

Furan (9.0 mmol, 612.6 mg, 654.5 µl) was dissolved in THF (4.5 mL) and the solution was cooled down to -40 ºC. ^{n}BuLi (8.5 mmol) was added slowly. Then the solution was allowed to reach room temperature, stirred for 3 h and diluted with 4.4 mL of THF to reach a final concentration of 0.6M.

[1] Raczko, J.; Golebiowski, A.; Krajewski, J. W.; Gluzinski, P.; Jurczak, J. *Tetrahedron Lett.* **1990**, *31*, 3797.

C. 2-Methoxymethoxy-phenyllithium[2]

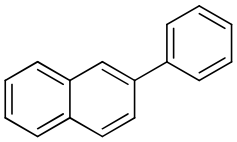
In a dry Schlenk flask (methoxymethoxy)benzene (1.0 mmol, 138 mg) was dissolved in dry THF (3 mL) and the solution was cooled down to -78 ºC. ^{t}BuLi (1 equiv) was added slowly and the solution was stirred for 1 h. Then the solution was allowed to reach room temperature.

D. 2-Methoxy-1-naphthyllithium

In a dry Schlenk flask 1-bromo-2-methoxynaphthalene (1.8 mmol, 427 mg) was dissolved in dry THF (0.9 mL) and slowly added (flow rate: 8 ml/h) to a solution of ^{n}BuLi (1.6 M in hexane, 1.05 equiv.) at -10 °C. The solution was then stirred for 30 min. and allowed to reach room temperature. The solution was diluted with 1 ml of toluene to reach a final concentration of 0.6M.

Data of Compounds 2a-2s, 10

Physical data for known compounds were identical in all respects to those previously reported (references are given).



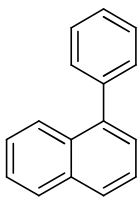
2-Phenylnaphthalene (2a):[3]

CAS Registry Number: 612-94-2.

Synthesized using catalytic systems A and B with 2-chloronaphthalene (0.3 mmol, 49 mg) and 225 µL of PhLi (1.8 M solution in dibutylether) diluted with 500 µL of THF.

Catalytic system A: Reaction carried out at room temperature. Flow rate of PhLi solution = 0.5 mL/h. White solid obtained after column chromatography (SiO_2, *n*-pentane/EtOAc 100:1), 54 mg, 88% yield.

Catalytic system B: Reaction carried out at room temperature in 2 mL of toluene. Flow rate of PhLi solution = 1 mL/h. White solid obtained after column chromatography, 57 mg, 93% yield.



1-Phenylnaphthalene (2b):[4]

CAS Registry Number: 605-02-7

Synthesized using catalytic systems A and B with 1-chloronaphthalene (0.3 mmol, 49 mg) and 225 µL of PhLi (1.8 M solution in dibutylether) diluted with 500 µL of THF.

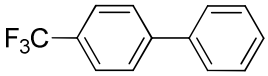
---

[2] Vo, C. T.; Mitchell, T. A.; Bode, J. W. *J. Am. Chem. Soc.* **2011**, *133*, 14082.

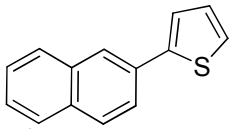
[3] Giannerini, M.; Fañanás-Mastral, M.; Feringa, B. L. *Nature Chem.* **2013**, doi:10.1038/nchem.1678.

[4] (a) Katakoa, N.; Shelby, Q.; Stambuli, J.P.; Hartwig, J.F. *J. Org. Chem*. **2002**, *67*, 5553.

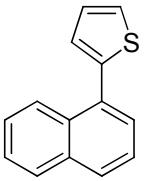
Catalytic system A: Reaction carried out at room temperature. Flow rate of PhLi solution = 0.5 mL/h. White solid obtained after column chromatography (SiO_2, *n*-pentane/EtOAc 100:1), 56 mg, 91% yield.
Catalytic system B: Reaction carried out at room temperature in 2 mL of toluene. Flow rate of PhLi solution = 1 mL/h. White solid obtained after column chromatography, 60 mg, 98% yield.
The reaction performed with 10 mmol (1.63 g) of substrate in the presence of 1 mol% of Pd_2dba_3 and 4 mol% of **L3** afforded product **2b** in 92% yield. Toluene = 30 mL. PhLi (8.3 mL, 1.8 M solution in dibutylether) diluted with 16.6 mL of THF. Flow rate of PhLi solution = 3 mL/h.



4-(Trifluoromethyl)-1,1'-biphenyl (2c):[5]
CAS Registry Number: 398-36-7
Synthesized using catalytic systems A and B with 1-chloro-4-(trifluoromethyl)benzene (0.3 mmol, 54 mg) and 225 µL of PhLi (1.8 M solution in dibutylether) diluted with 500 µL of THF.
Catalytic system A: Reaction carried out at room temperature. Flow rate of PhLi solution = 0.5 mL/h. White solid obtained after column chromatography (SiO_2, *n*-pentane/Et_2O 100:1), 59 mg, 89% yield.
Catalytic system B: Reaction carried out at room temperature in 2 mL of toluene. Flow rate of PhLi solution = 1 mL/h. White solid obtained after column chromatography, 63 mg, 95% yield.



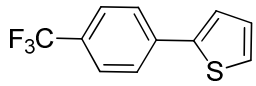
2-(Naphthalen-2-yl)thiophene (2d):[6]
CAS Registry Number: 16939-09-6
Synthesized using catalytic systems A with 2-chloronaphthalene (0.3 mmol, 49 mg) and 750 µL of thienyllithium (0.6M). White solid obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 52 mg, 82% yield.



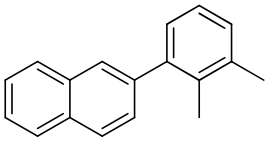
2-(Naphthalen-1-yl)thiophene (2e):[7]

[5] Guha, N. R.; Reddy, C. B.; Aggarwal, N.; Sharma, D.; Shil, A. K.; Das, B. P. *Adv. Synth. Catal*. **2012**, *354*, 2911.
[6] Bolliger, J. L.; Frech, C. M.. *Adv. Synth. Cat*. **2010**, *352*, 1075.
[7] Cahiez, G.; Moyeux, A.; Gager, O.; Poizat, M. *Adv. Synth. Cat*. **2013**, *355*, 790

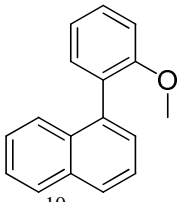
CAS Registry Number: 4632-51-3.
Synthesized using catalytic systems A with 1-chloronaphthalene (0.3 mmol, 49 mg) and 750 µL of thienyllithium (0.6M). Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 55 mg, 87% yield.



2-(4-(Trifluoromethyl)phenyl)thiophene (2f):[8]
CAS Registry Number: 115933-15-8.
Synthesized using catalytic systems A with 1-chloro-4-(trifluoromethyl)benzene (0.3 mmol, 54 mg) and 750 µL of thienyllithium (0.6M). White solid obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 57 mg, 83% yield.

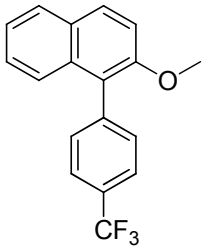


2-(2,3-Dimethylphenyl)naphthalene (2g).[9]
CAS Registry Number: 382151-52-2.
Synthesized using catalytic systems B with 2-chloronaphthalene (0.3 mmol, 49 mg) and 725 µL of 2,3-dimethyl-phenyllithium (0.6M). Reaction carried out at room temperature in 2 mL of toluene. Flow rate of 2,3-dimethyl-phenyllithium solution = 1 mL/h. White solid obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 62 mg, 89% yield.

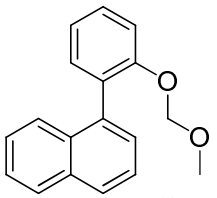


1-(2-Methoxyphenyl)naphthalene (2h).[10]
CAS Registry Number: 93321-11-0.
Synthesized using catalytic systems A with 1-chloronaphthalene (0.3 mmol, 49 mg) and 725 µL of 2-methoxy-phenyllithium (0.6M). Reaction carried out at room temperature. Flow rate of PhLi solution = 0.5 mL/h. White solid obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 59 mg, 84% yield.

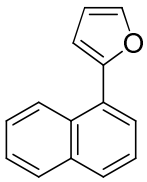
[8] Shi, S.; Zhang, Y.; *Green Chem.* **2008**, *10*, 868.
[9] Yonehara, F.; Kido, Y.; Sugimoto, H.; Morita, S.; Yamaguchi, M. *J. Org. Chem.* **2003**, *68*, 6752.
[10] Song, C.; Ma, Y.; Chai, Q.; Ma, C.; Jiang, W.; Andrus, M. B. *Tetrahedron* **2005**, *61*, 7438–7446.



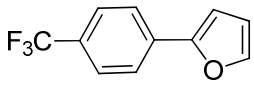
2-Methoxy-1-(4-(trifluoromethyl)phenyl)naphthalene (2i):[11]
CAS Registry Number: 922511-77-1.
Synthesized using catalytic systems A with 1-chloro-4-(trifluoromethyl)benzene (0.3 mmol, 54 mg) and 725 µL of 2-methoxy-1-naphthyllithium (0.6M). Reaction carried out at room temperature. Flow rate of PhLi solution = 0.5 mL/h. White solid obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 70 mg, 77% yield.



1-(2-(methoxymethoxy)phenyl)naphthalene (2j):[12]
CAS Registry Number: 141362-07-4.
Synthesized using catalytic systems A with 1-chloronaphthalene (0.3 mmol, 49 mg) and 1500 µL of 2-Methoxy-phenyllithium (0.3M). Reaction carried out at room temperature. Flow rate of PhLi solution = 0.5 mL/h. Waxy solid obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:2), 66 mg, 83% yield.



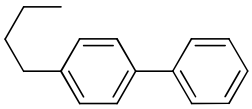
2-(Naphthalen-1-yl)furan (2k):[13]
CAS Registry Number: 51792-32-6.
Synthesized using catalytic systems A with 1-chloronaphthalene (0.3 mmol, 49 mg) and 725 µL of furyllithium (0.6M). Pale yellow oil obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 56 mg, 96% yield.



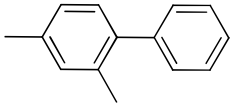
2-(4-(Trifluoromethyl)phenyl)furan (2l):[14]

[11] Li, H.; Wu, Y.; Yan, W. *J. Organomet. Chem.* **2006**, *691*, 5688.
[12] Wawrzyniak, P.; Heinicke, J. *Tetrahedron Lett.* **2006**, *47*, 8921.
[13] Molander, G. A.; Beaumard, F. *Org. Lett.* **2010,** *12*, 4022.

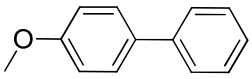
CAS Registry Number: 214463-10-2.
Synthesized using catalytic systems A with 1-chloro-4-(trifluoromethyl)benzene (0.3 mmol, 54 mg) and 725 µL of furyllithium (0.6M). White solid obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 49 mg, 77% yield.



4-Butyl-1,1'-biphenyl (2m):[15]
CAS Registry Number: 37909-95-8.
Synthesized using catalytic systems A and B with 1-butyl-4-chlorobenzene (0.3 mmol, 51 mg) and 225 µL of PhLi (1.8 M solution in dibutylether) diluted with 500 µL of THF.
Catalytic system A: Reaction carried out at 35°C. Flow rate of PhLi solution = 0.2 mL/h. White solid obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 54 mg, 86% yield.
Catalytic system B: Reaction carried out at 40°C in 1 mL of toluene. Flow rate of PhLi solution = 0.2 mL/h. Colorless oil obtained after column chromatography, 53 mg, 84% yield.



2,4-Dimethyl-1,1'-biphenyl (2n):[16]
CAS Registry Number: 4433-10-7.
Synthesized using catalytic systems A and B with 1-chloro-2,4-dimethylbenzene (0.3 mmol, 42 mg) and 225 µL of PhLi (1.8 M solution in dibutylether) diluted with 500 µL of THF. **Catalytic system A:** Reaction carried out at 35°C. Flow rate of PhLi solution = 0.2 mL/h. White solid obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 44 mg, 80% yield.
Catalytic system B: Reaction carried out at 40°C in 1 mL of toluene. Flow rate of PhLi solution = 0.2 mL/h. Colorless oil obtained after column chromatography, 45 mg, 82% yield.



4-Methoxybiphenyl (2o):[3]
CAS Registry Number: 613-37-6.
Synthesized using catalytic systems A and B with 1-chloro-4-methoxybenzene (0.3 mmol, 43 mg) and 225 µL of PhLi (1.8 M solution in dibutylether) diluted with 500 µL of THF. **Catalytic system A:** Reaction carried out at 40°C. Flow rate of PhLi solution =

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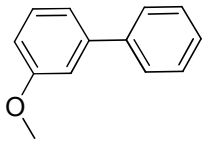
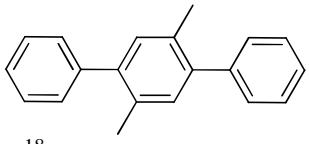
[14] Denmark, S. E.; Baird, J. D. *Org. Lett*. **2006,** *8*, 793.
[15] Littke, A. F.; Schwarz, L.; Fu, G. C. *J. Am. Chem. Soc.* **2002**, *124*, 6343.
[16] Zim, D.; Gruber, A. S.; Ebeling, G.; Dupont, J.; Monteiro, A. L. *Org. Lett*. **2000,** *2*, 2881.

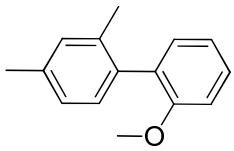
0.2 mL/h. White solid obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 52 mg, 94% yield.
Catalytic system B: Reaction carried out at 40°C in 1 mL of toluene. Flow rate of PhLi solution = 0.2 mL/h. Colorless oil obtained after column chromatography, 34 mg, 62% yield.



3-Methoxy-1,1'-biphenyl (2p).[17]
CAS Registry Number: 2113-56-6.
Synthesized using catalytic systems A with 1-chloro-3-methoxybenzene (0.3 mmol, 43 mg) and 225 µL of PhLi (1.8 M solution in dibutylether) diluted with 500 µL of THF. Reaction carried out at 40°C. Flow rate of PhLi solution = 0.2 mL/h. Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 42 mg, 76% yield.

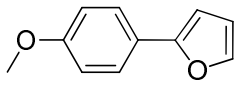


2',5'-Dimethyl-*p*-terphenyl (2q):[18]
CAS Registry Number: 20260-22-4.
Synthesized using catalytic systems A with 1-chloro-4-methoxybenzene (0.3 mmol, 53 mg) and 500 µL of PhLi (1.8 M solution in dibutylether) diluted with 1.5 mL of THF. Reaction carried out at 40°C. Flow rate of PhLi solution = 0.2 mL/h. Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 62 mg, 80% yield.

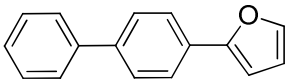


2'-Methoxy-2,4-dimethyl-1,1'-biphenyl (2r).
Synthesized using catalytic systems A with 2,4-dimethylbenzene (0.3 mmol, 42 mg) and 725 µL of 2-methoxy-phenyllithium (0.6M). Reaction carried out at 35°C. Flow rate of PhLi solution = 0.2 mL/h. Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:1), 55 mg, 86% yield. . ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (td, *J* = 8.2, 1.8 Hz, 1H), 7.99 – 7.20 (m, 6H), 3.81 (s, 3H), 2.41 (s, 3H), 2.16 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 136.9, 136.6, 135.7, 131.2, 130.8, 130.5, 130.0, 128.4, 126.3, 120.4, 110.6, 55.4, 21.2, 19.9 ppm. EI-MS m/z (%) 212 (100).

[17] Mino, T.; Shirae, Y.; Sakamoto, M.; Fujita, T. *J. Org. Chem.* **2005**, *70*, 2191.
[18] K.-Nezhad, A.; Panahi, F. *J. Organomet. Chem*. **2012**, *717*, 146.



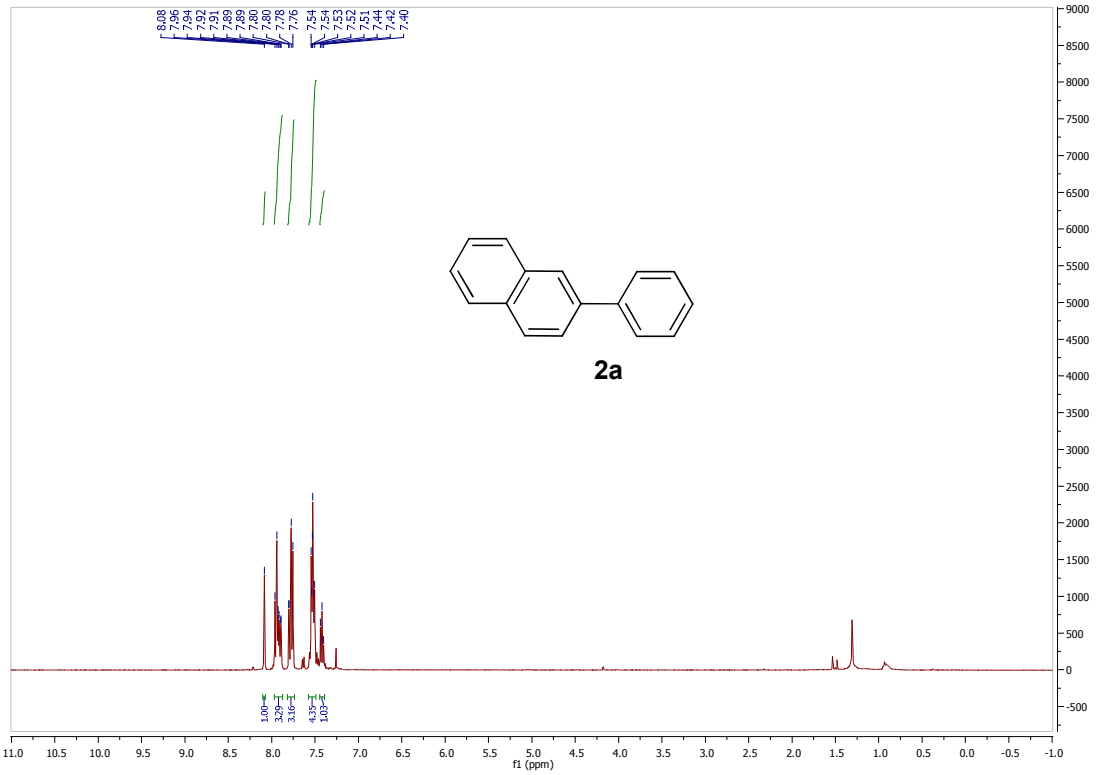
2-(4-Methoxyphenyl)furan (2s):[19]
CAS Registry Number: 17113-31-4.
Synthesized using catalytic systems A with 1-chloro-4-methoxybenzene (0.3 mmol, 43 mg) and 725 µL of furyllithium (0.6M). White solid obtained after column chromatography (SiO_2, *n*-pentane/ EtOAc 100:2), 51 mg, 80% yield.

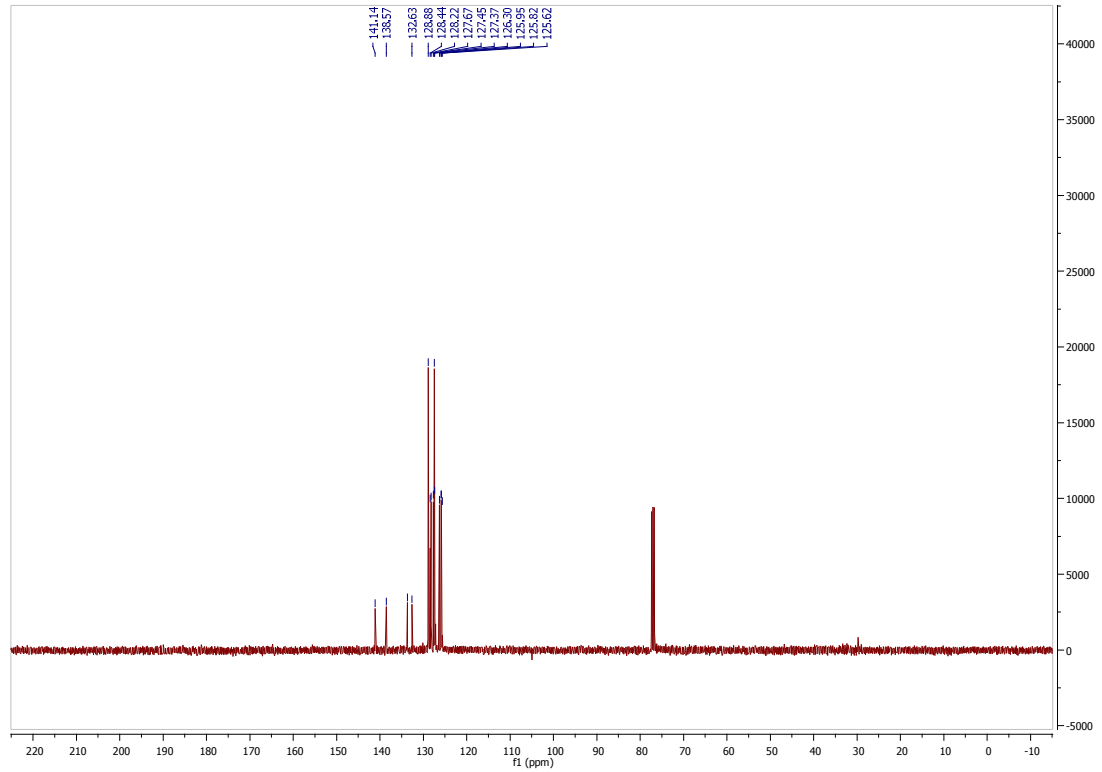


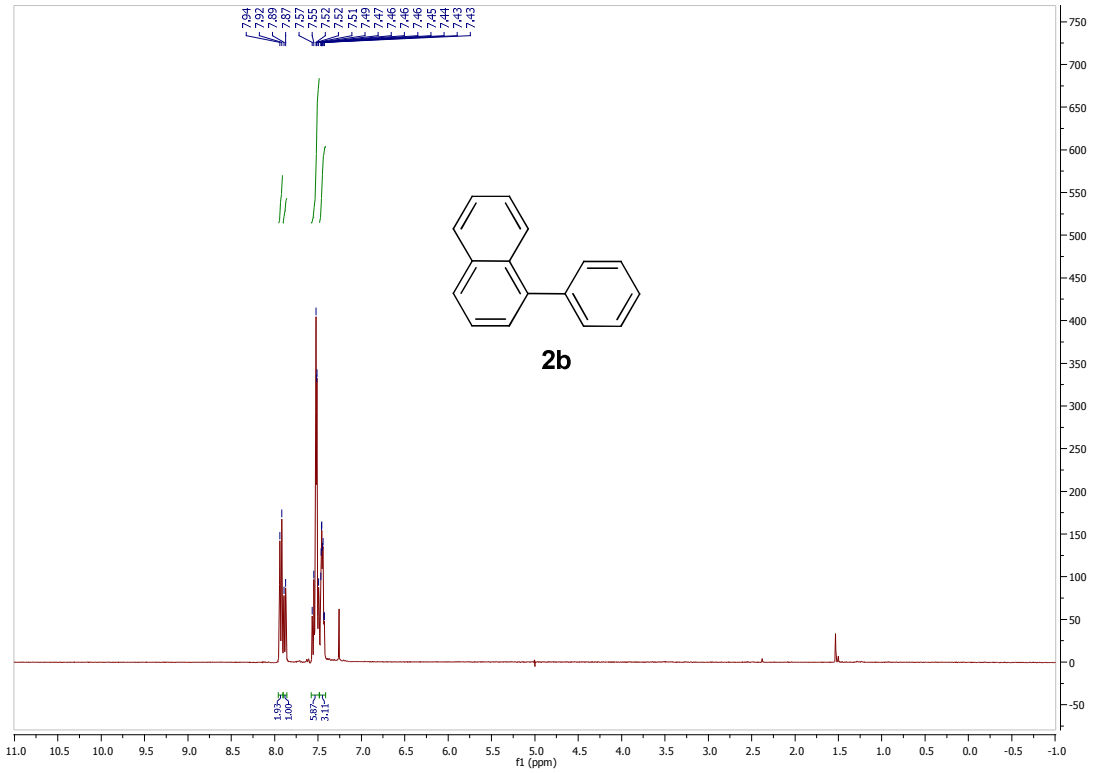
2-([1,1'-Biphenyl]-4-yl)furan (10):[20]
Synthesized using catalytic systems A with **9** (0.3 mmol, 57 mg) and 725 µL of furyllithium (0.6M). White solid obtained after column chromatography (SiO_2, *n*-pentane), 59 mg, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 8.4 Hz, 2H), 7.69 – 7.62 (m, 4H), 7.52 (d, J = 1.7 Hz, 1H), 7.48 (t, J = 7.6 Hz, 2H), 7.38 (t, J = 7.3 Hz, 1H), 6.72 (d, J = 3.3 Hz, 1H), 6.52 (dd, J = 3.3, 1.7, Hz 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.8, 142.2, 140.6, 140.0, 129.9, 128.8, 127.4, 126.9, 124.2, 111.8, 105.2 ppm. HRMS (ESI+, *m/z*): calcd for $C_{16}H_{13}O$ $[M+H]^+$: 221.09609; found: 221.09511.

[19] Naber, J. R.; Buchwald, S. L. *Adv. Synth. Cat*., **2008**, *350*, 957.
[20] Haner, J.; Jack, K.; Nagireddy, J.; Raheem, M. A.; Durham, R.; Tam, W. *Synthesis*, **2011**, 731.

^{1}H and ^{13}C NMR spectra



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7.87
7.57
7.55
7.52
7.52
7.51
7.49
7.47
7.46
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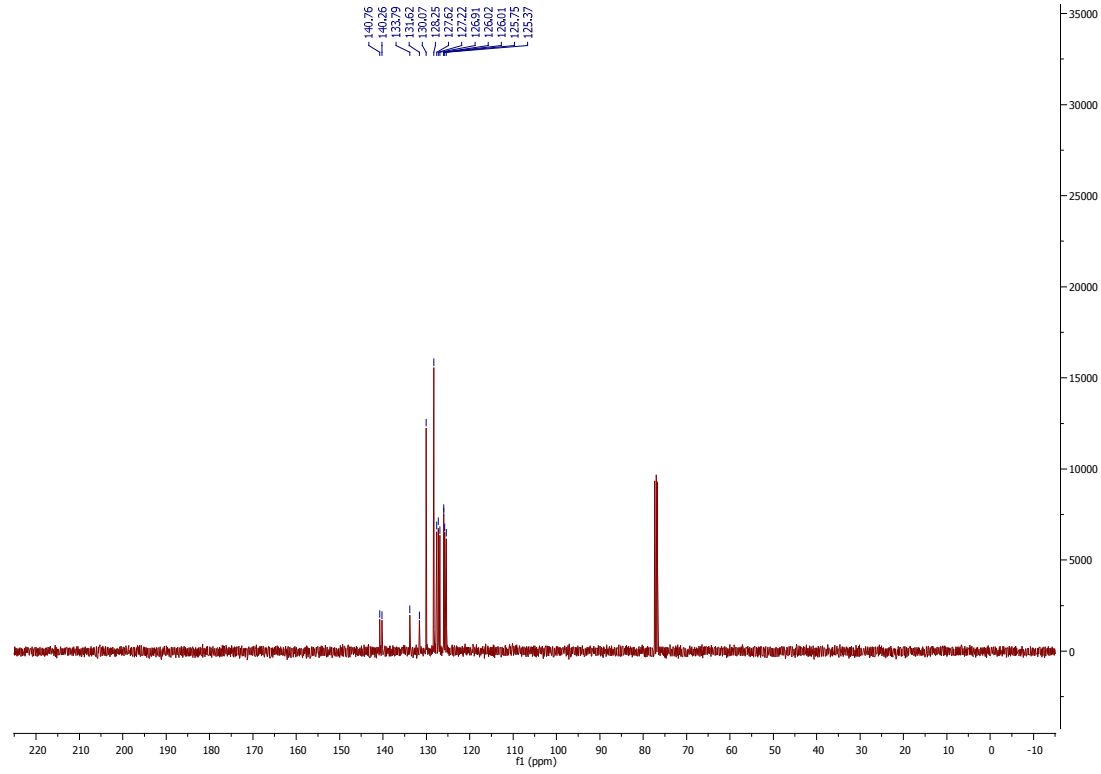
1.00
5.87
3.11
2b
f1 (ppm)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126.02
126.01
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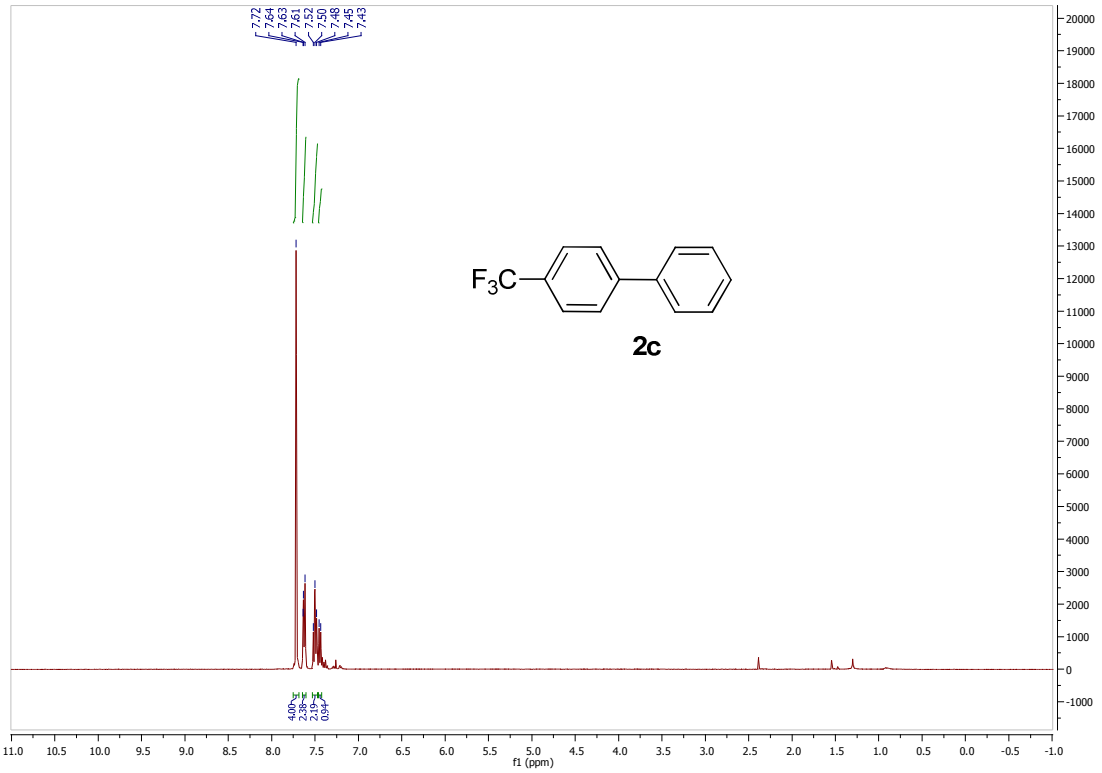
125.37
f1 (ppm)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7.63
7.61
7.52
7.50
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7.45
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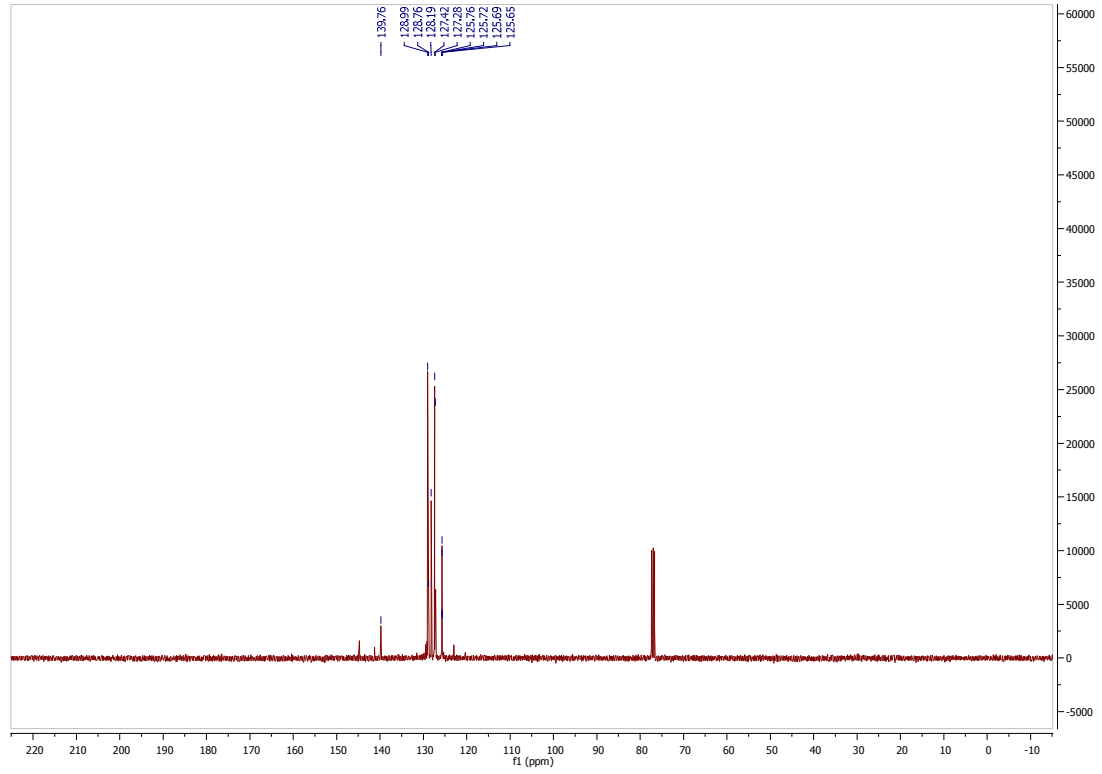
4.00
2.38
2.31
0.91
F3C
2c
f1 (ppm)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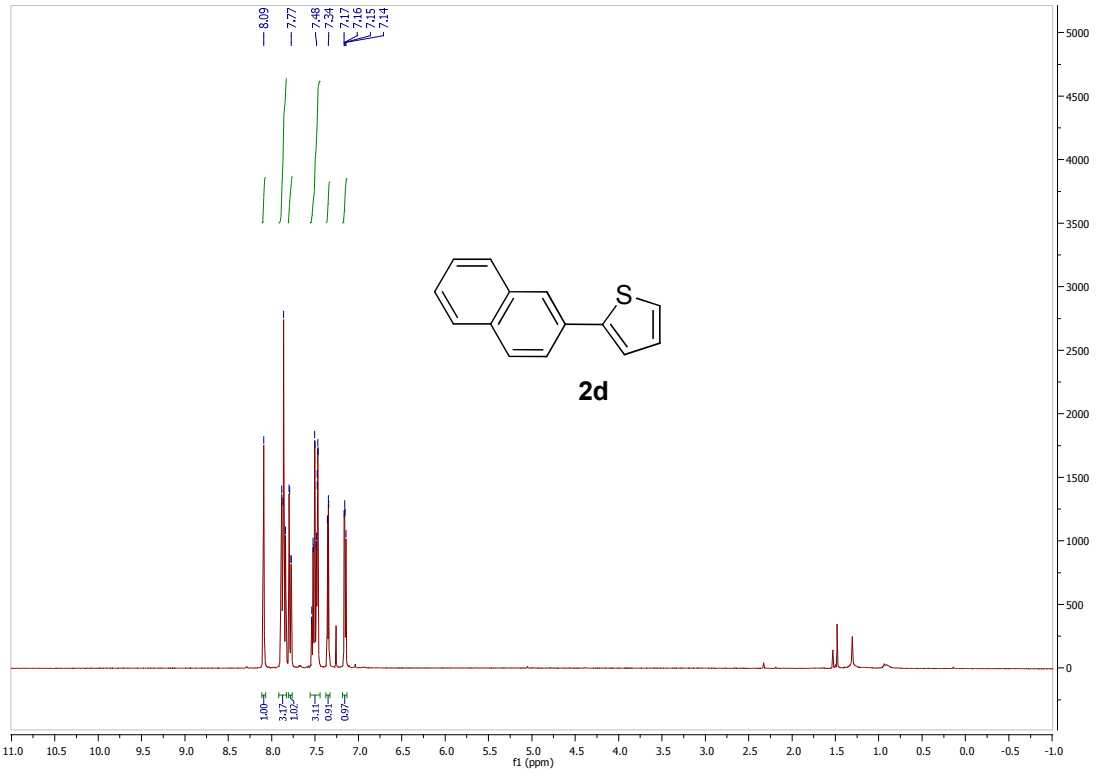
125.65
f1 (ppm)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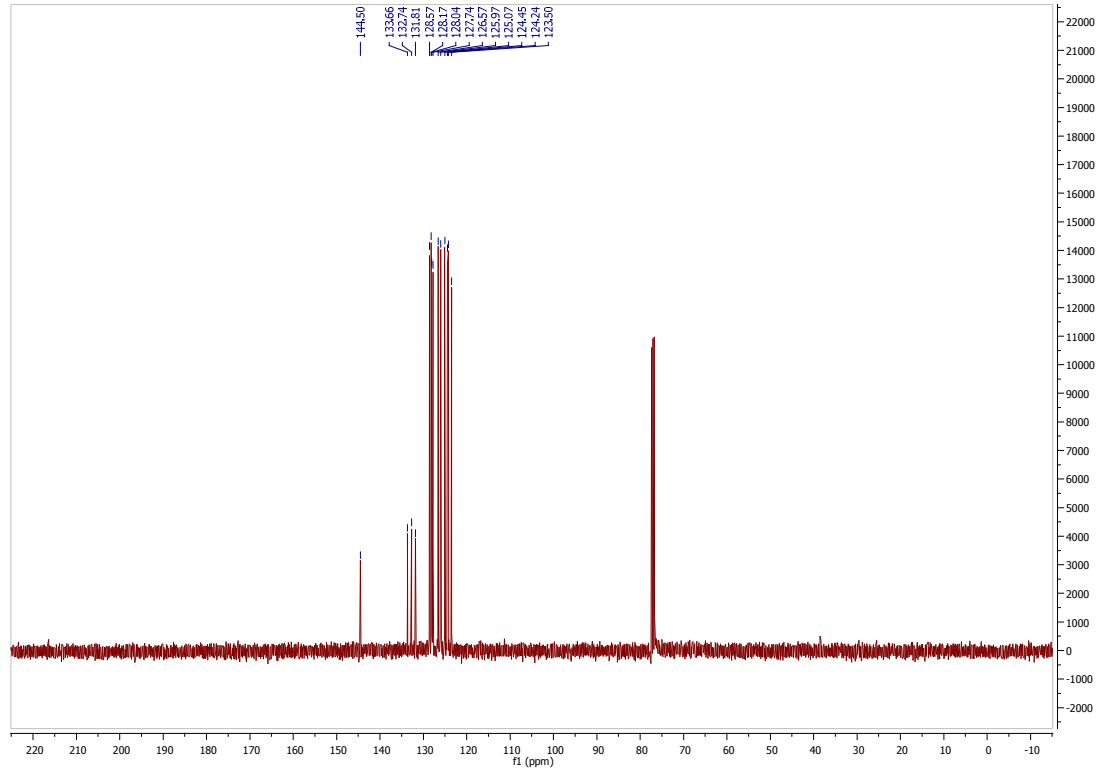
7.17
7.16
7.15
7.14
S
2d
1.00
3.17
1.02
3.11
0.91
0.97
f1 (ppm)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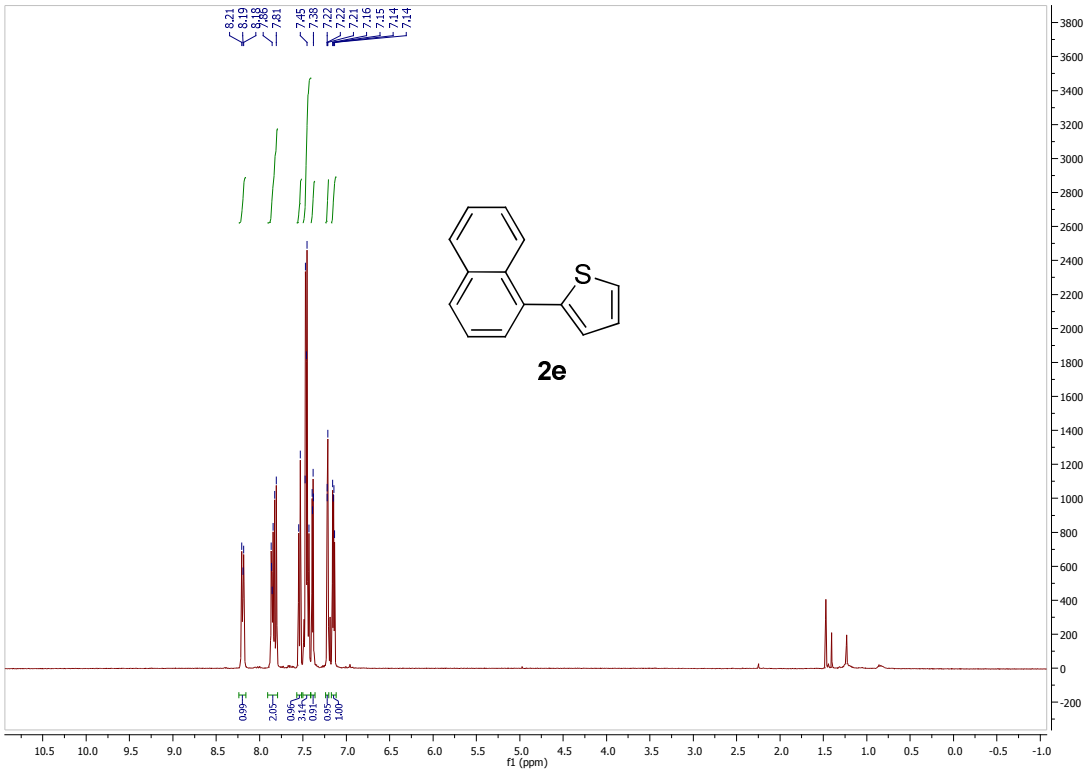
f1 (ppm)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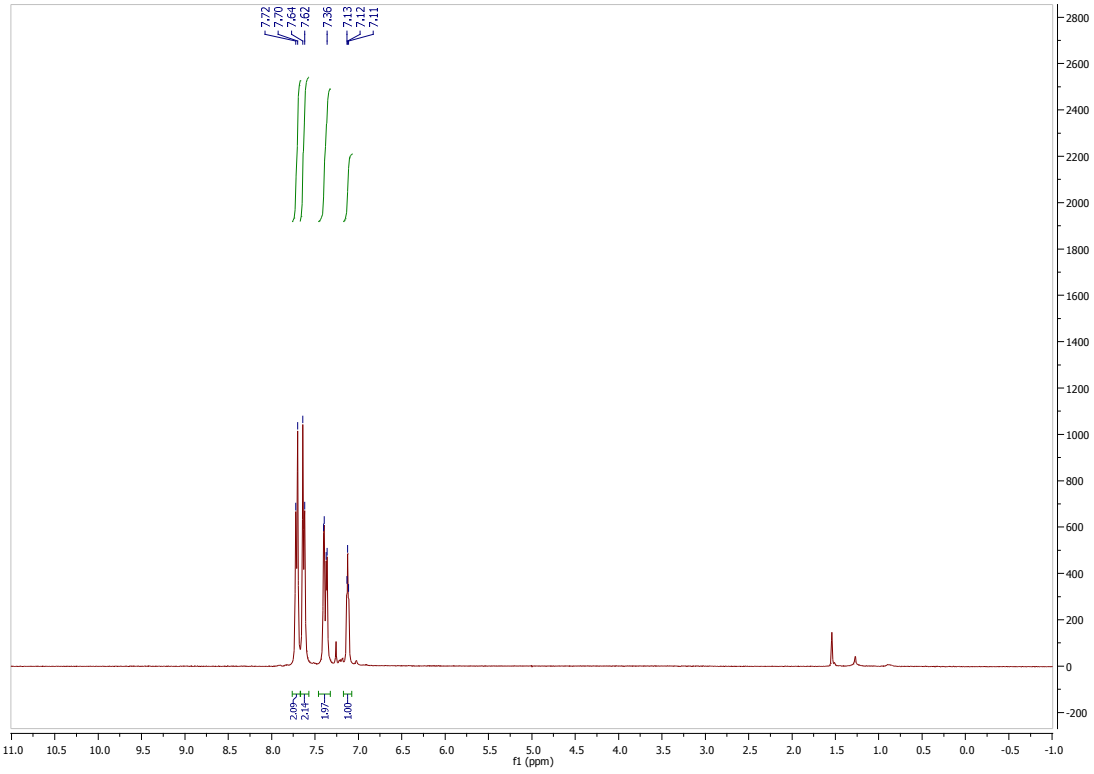
7.14
7.14
S
2e
f1 (ppm)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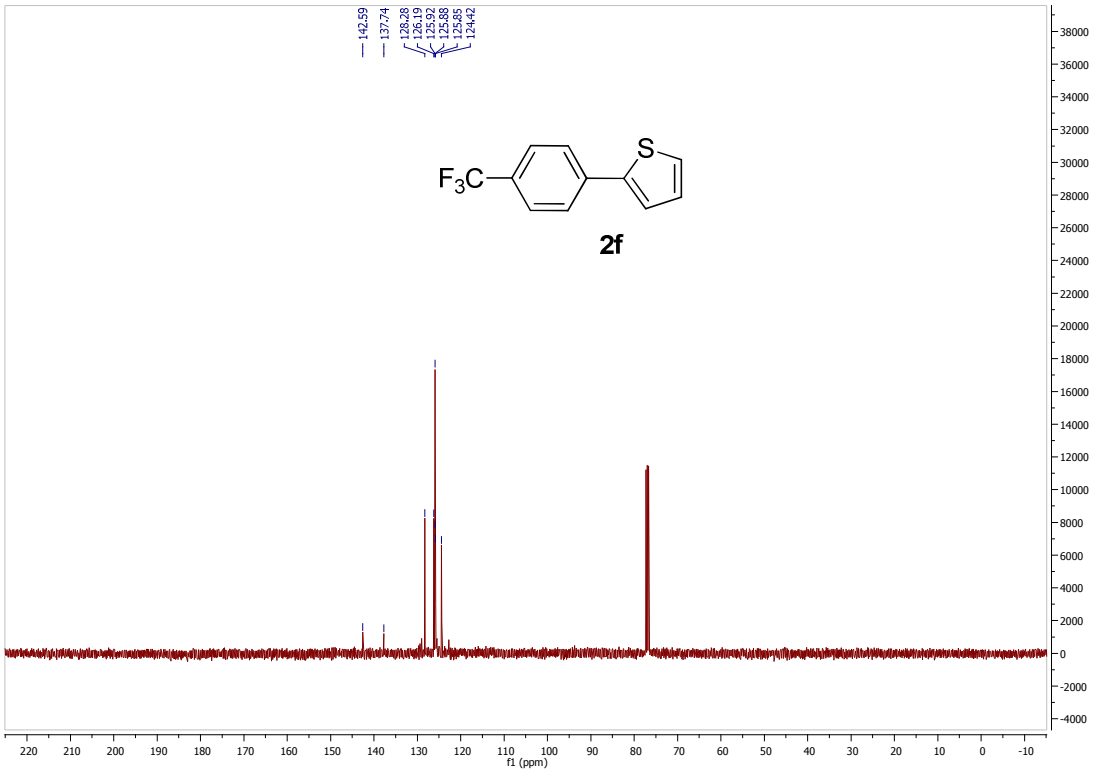
f1 (ppm)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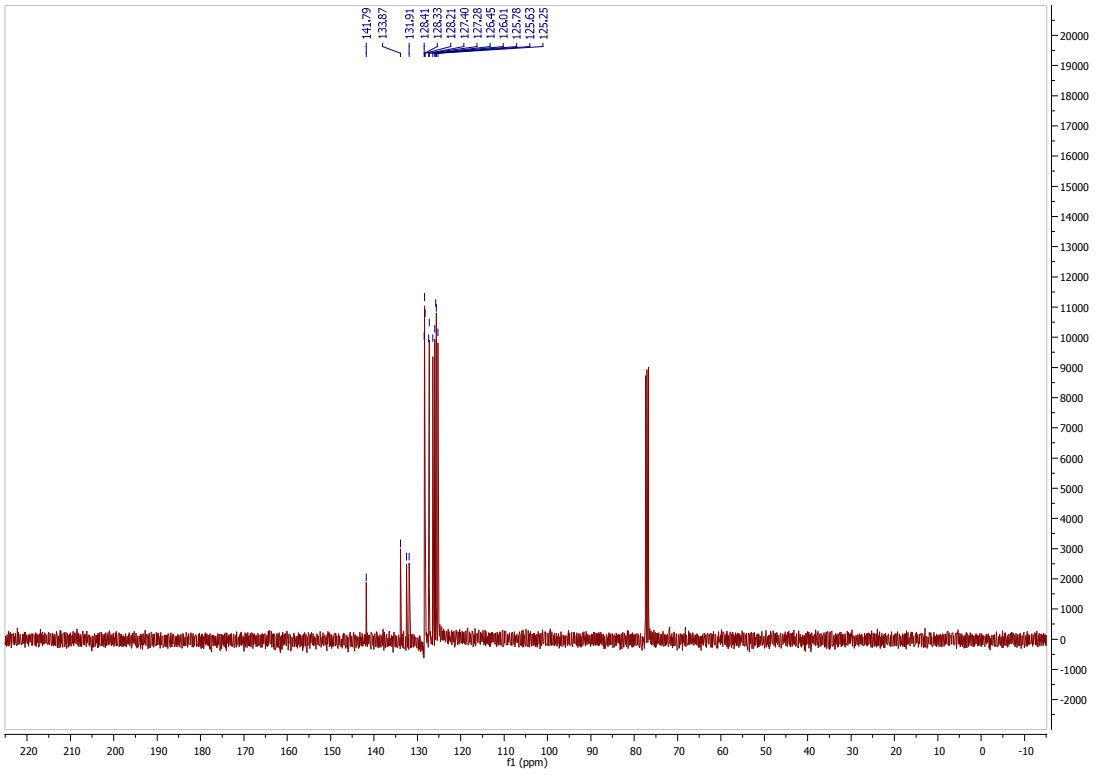
S
F3C
2f
f1 (ppm)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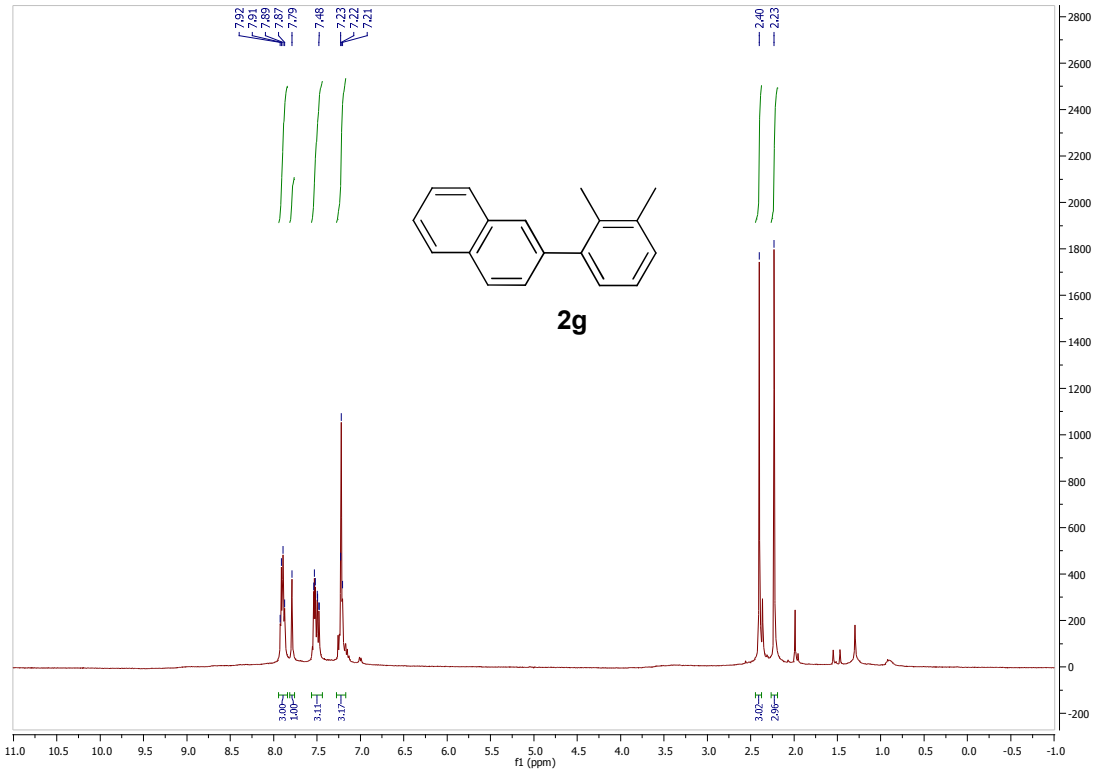
f1 (ppm)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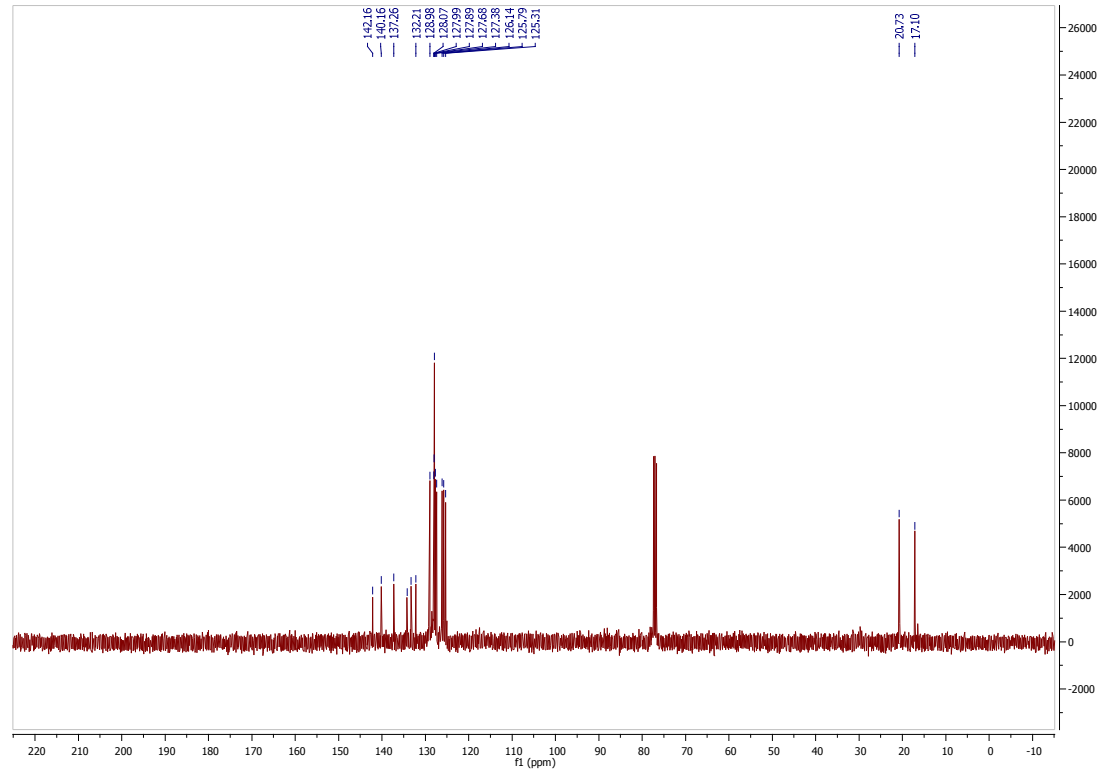
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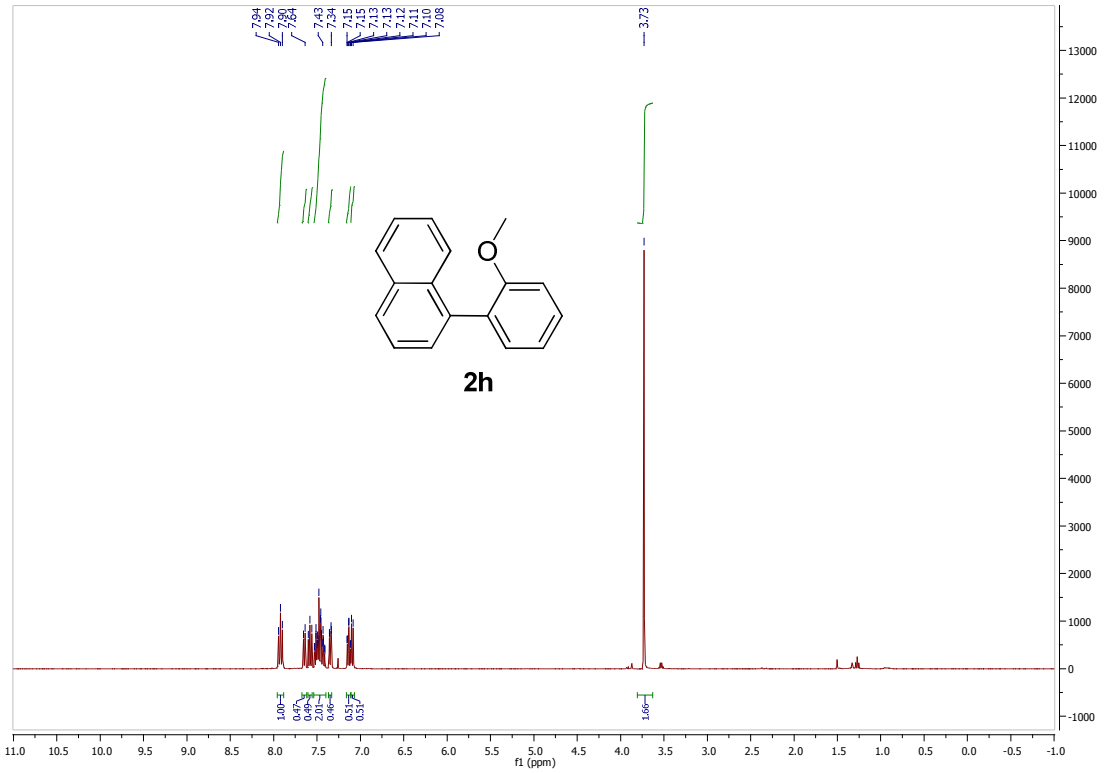
f1 (ppm)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7.12
7.11
7.10
7.08
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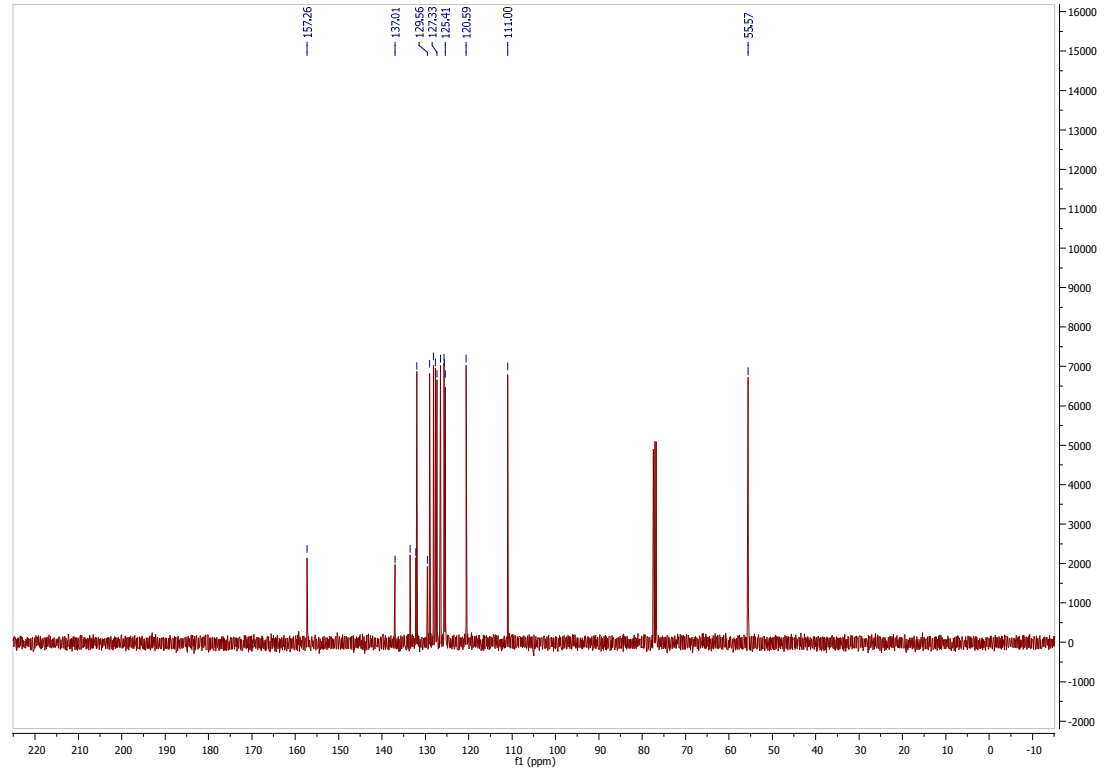
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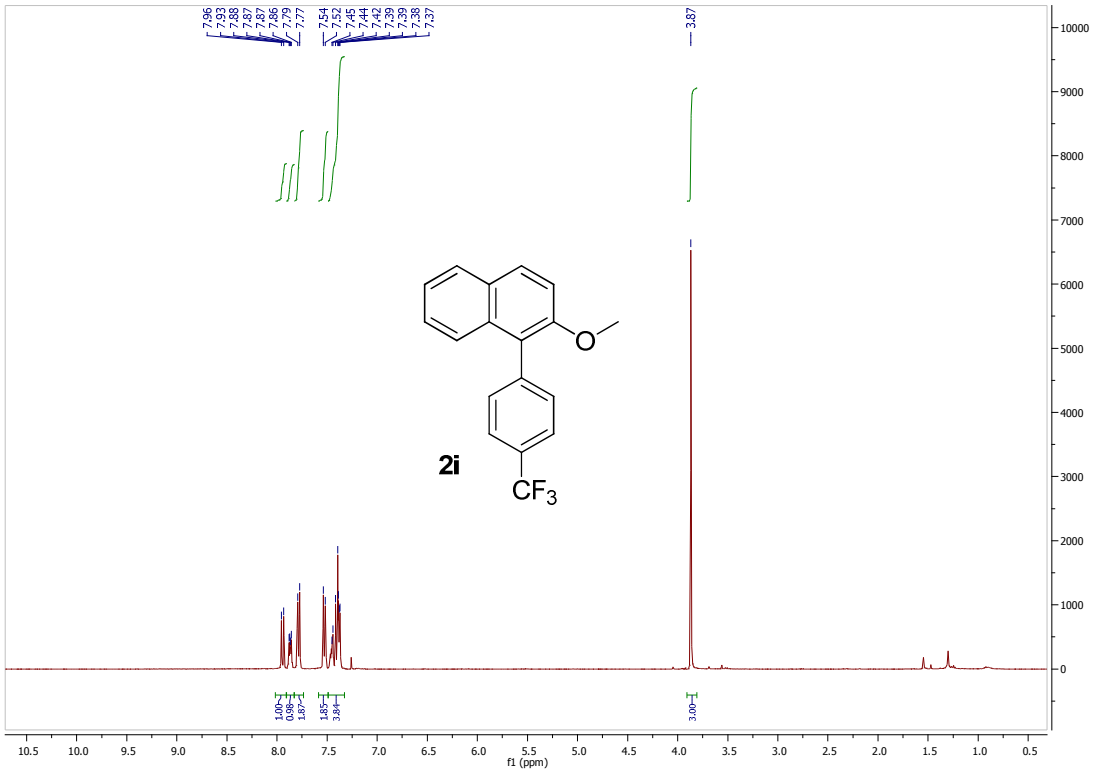
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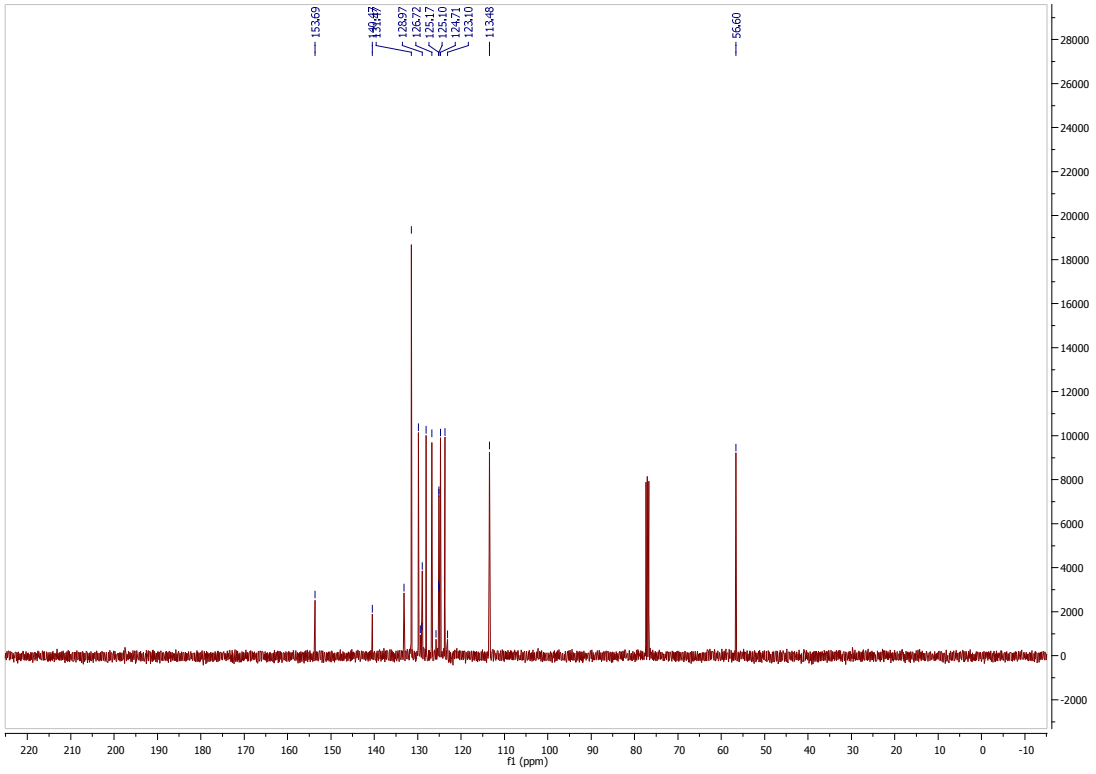
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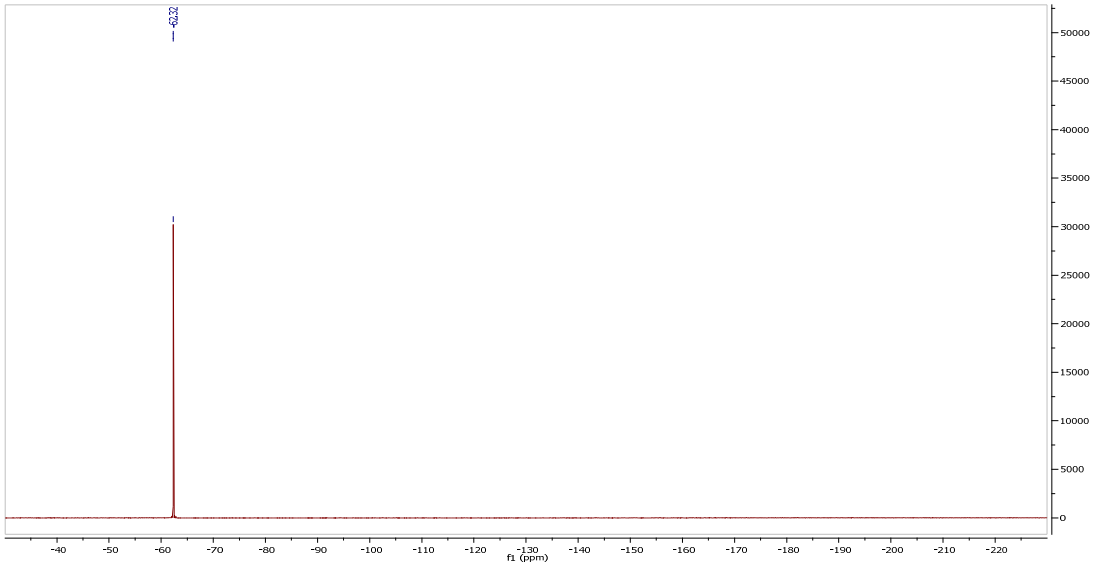
f1 (ppm)

^{19}F NMR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-190
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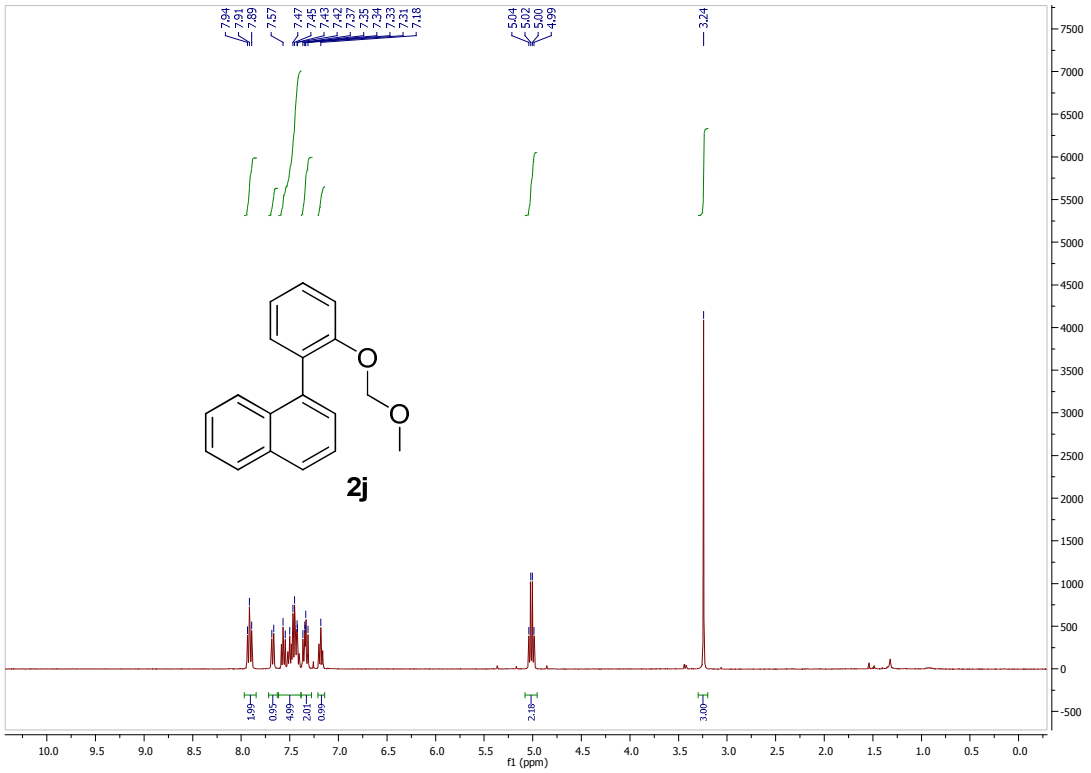
-210
-220
f1 (ppm)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7.18
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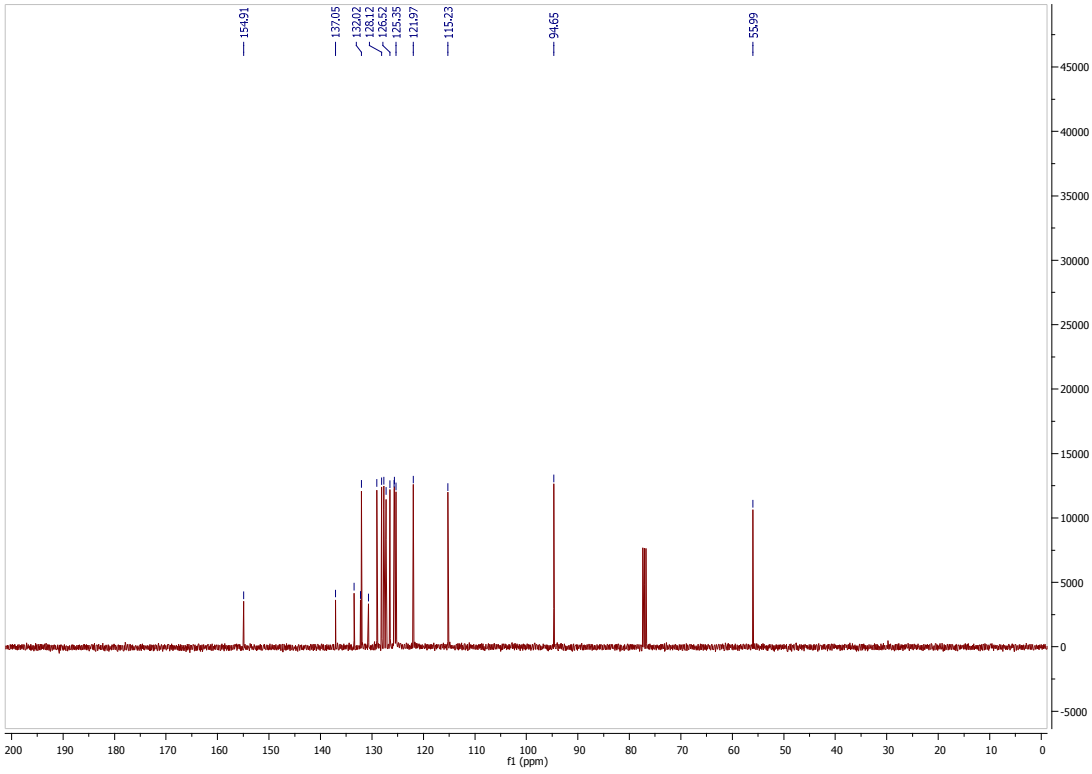
f1 (ppm)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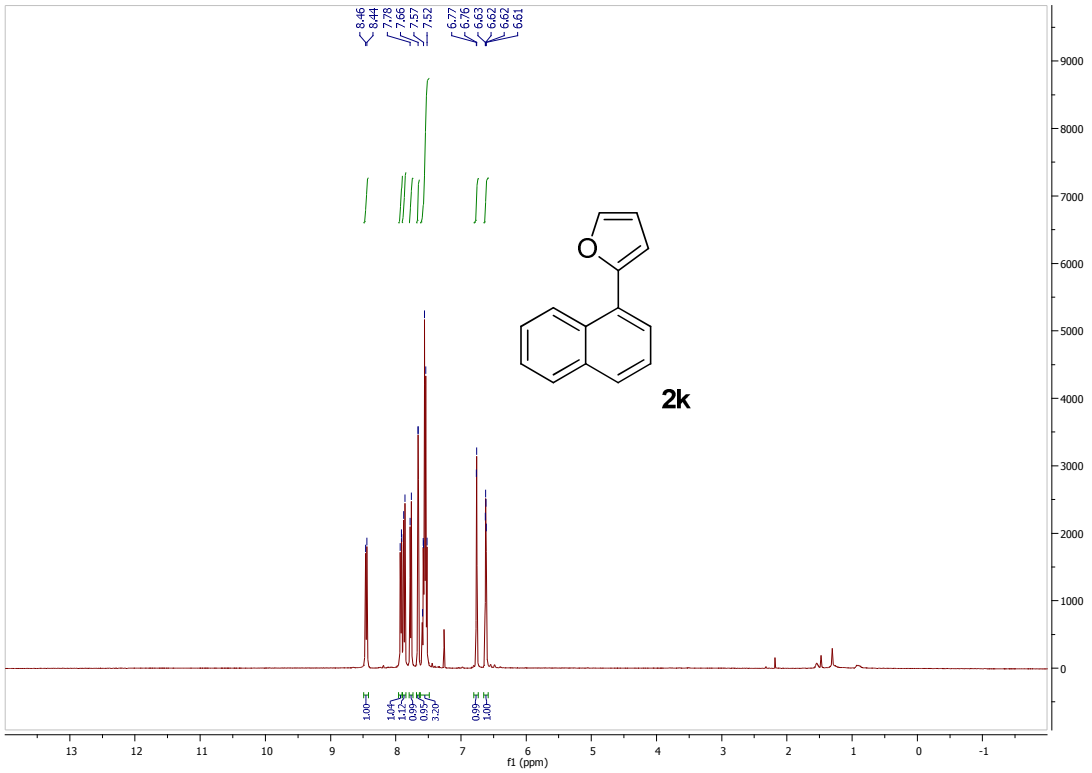
f1 (ppm)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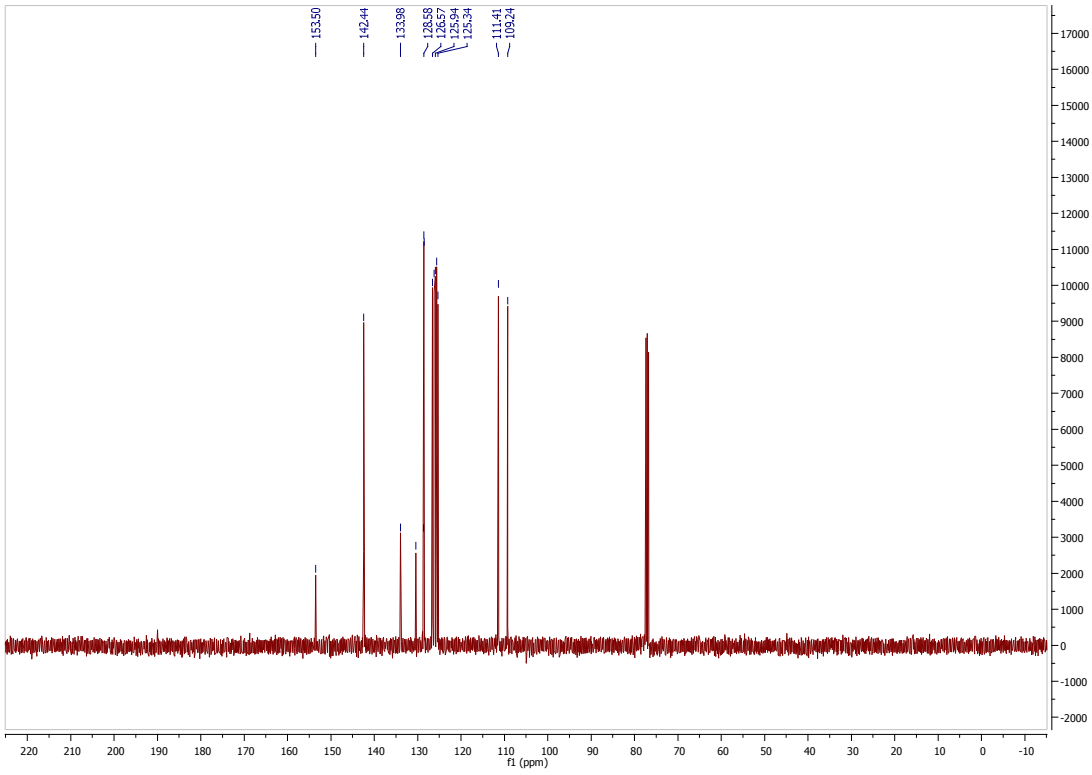
O
2k
f1 (ppm)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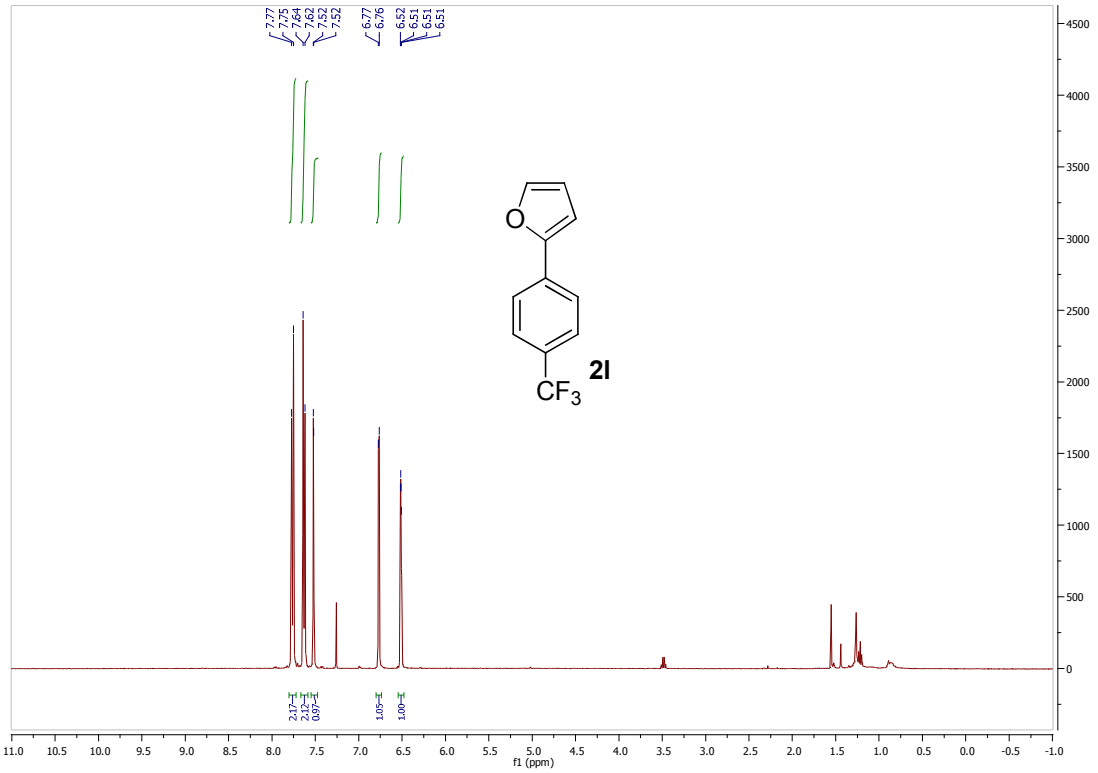
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2l
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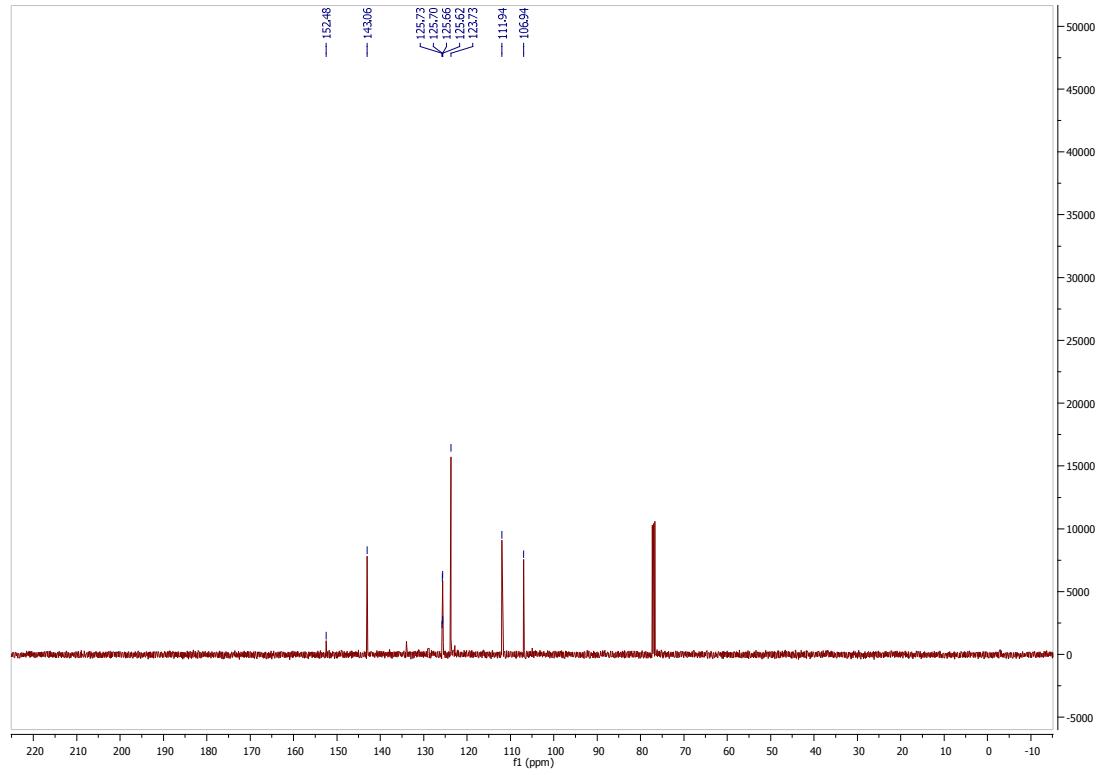
f1 (ppm)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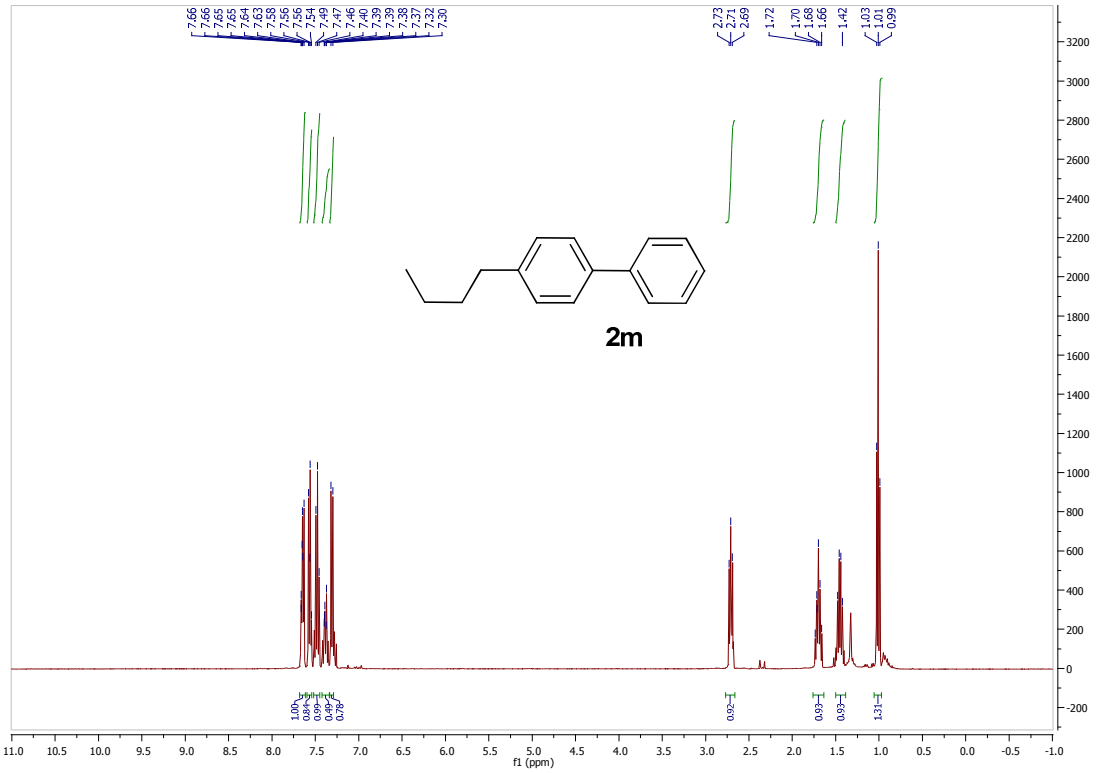
125.66
125.62
123.73
111.94
106.94
f1 (ppm)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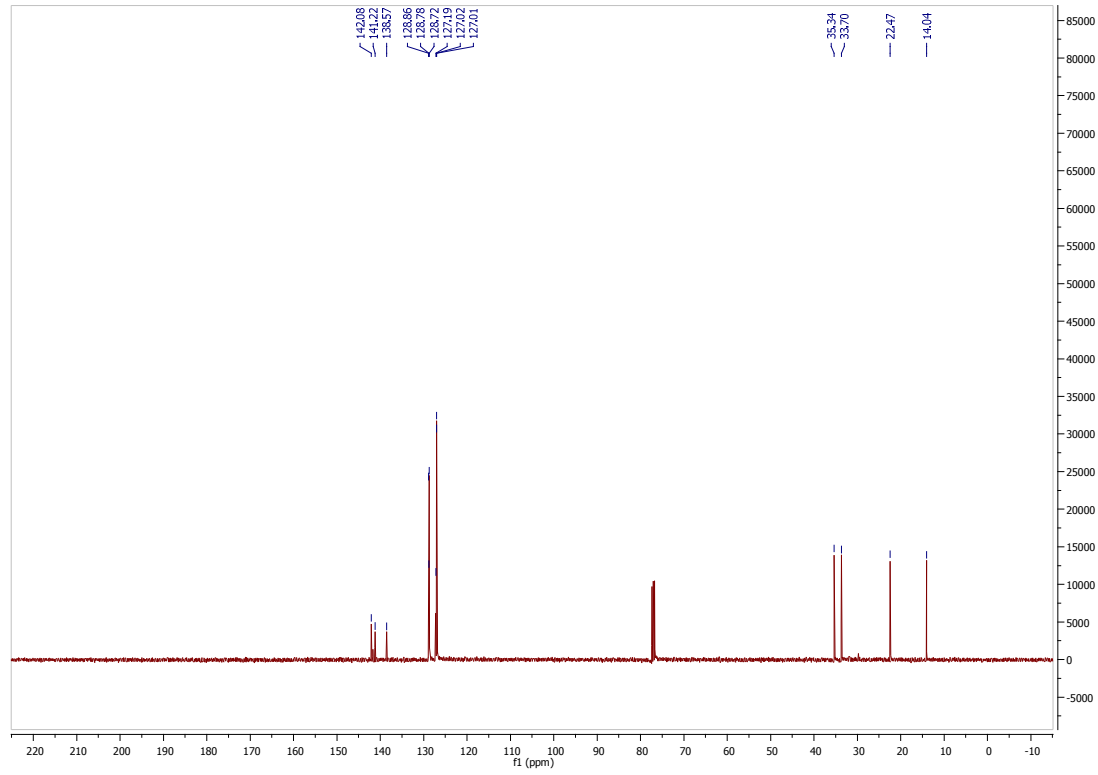
7.66
7.65
7.65
7.64
7.63
7.58
7.56
7.54
7.49
7.47
7.46
7.40
7.39
7.38
7.37
7.32
7.30
2.73
2.71
2.69
1.72
1.70
1.68
1.66
1.42
1.03
1.01
0.99
2m
1.00
0.84
0.95
0.48
0.70
0.92
0.99
0.93
1.31
f1 (ppm)


142.08
141.22
138.57
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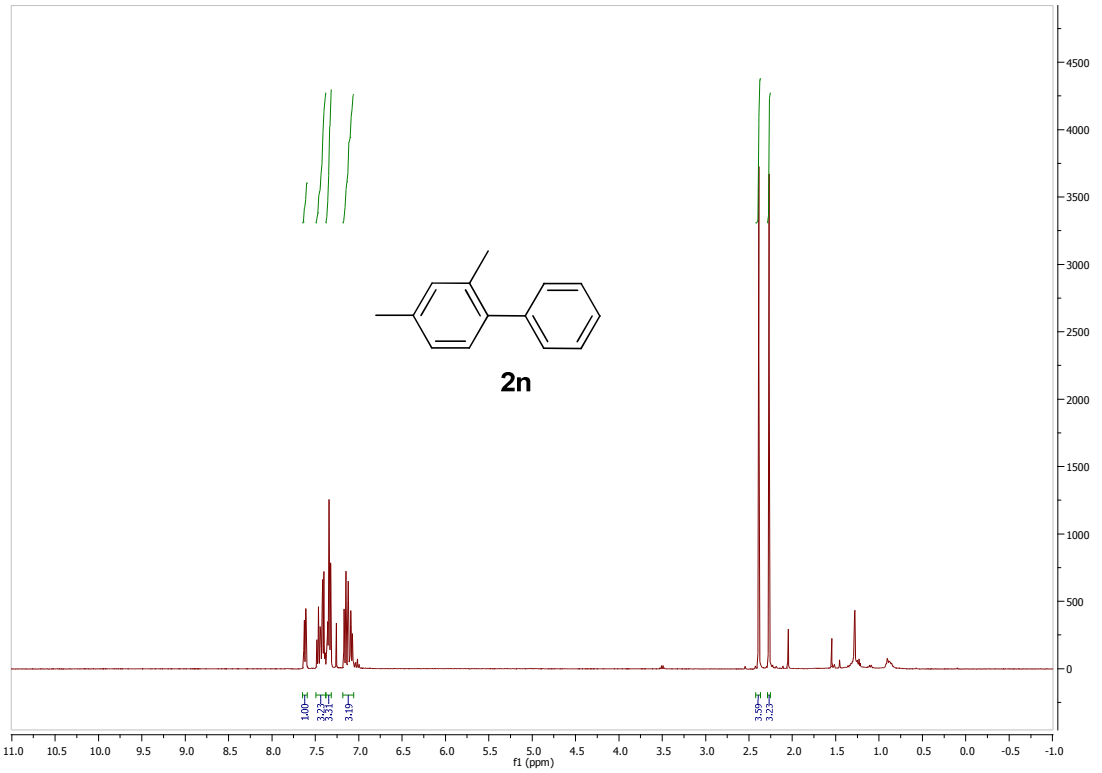
128.78
128.72
127.19
127.02
127.01
35.34
33.70
22.47
14.04
f1 (ppm)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3.23
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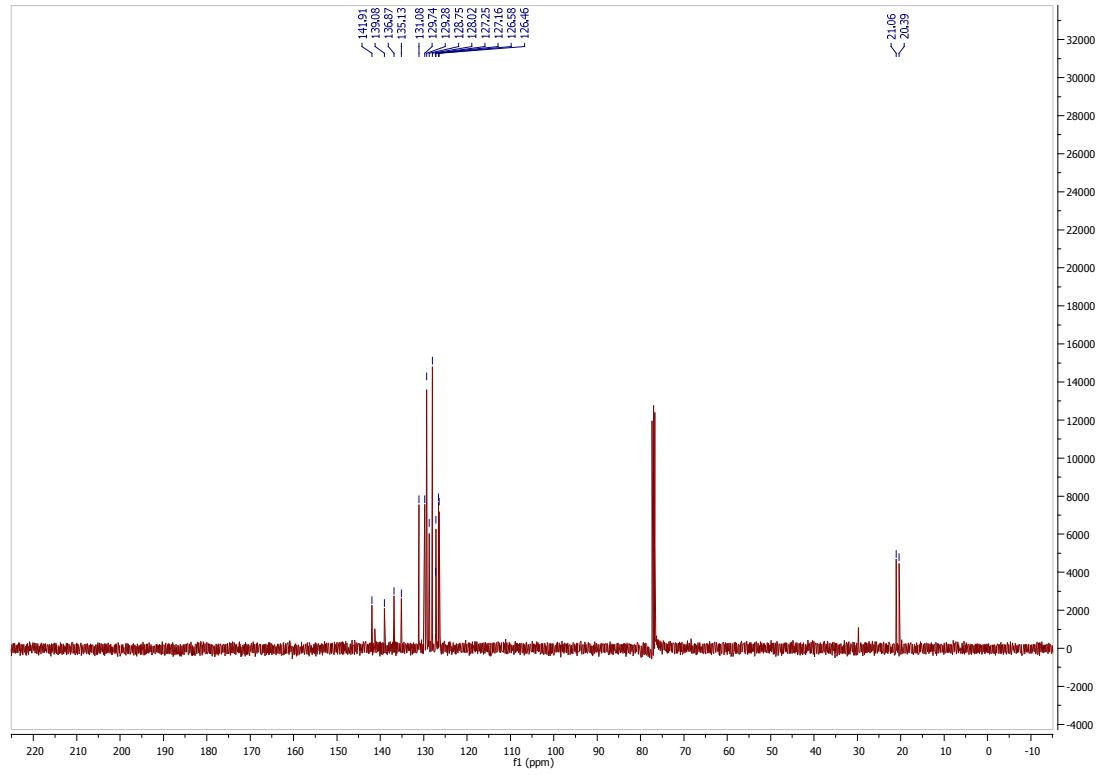
3.23
f1 (ppm)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139.08
136.87
135.13
131.08
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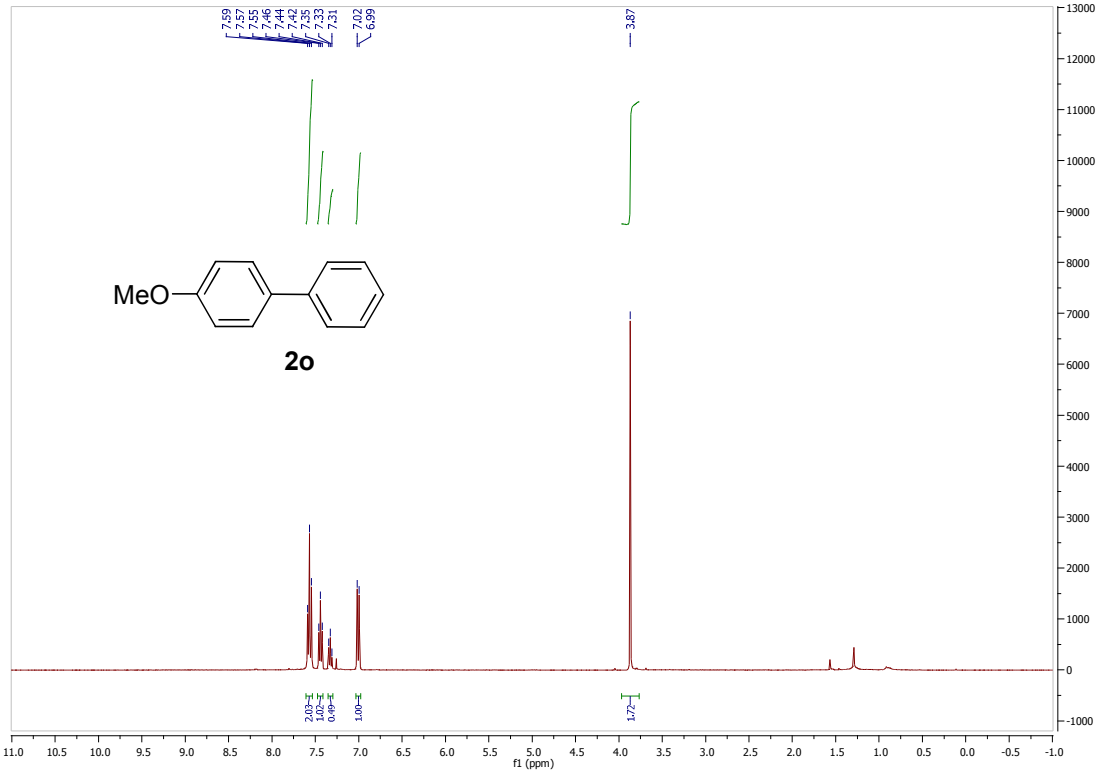
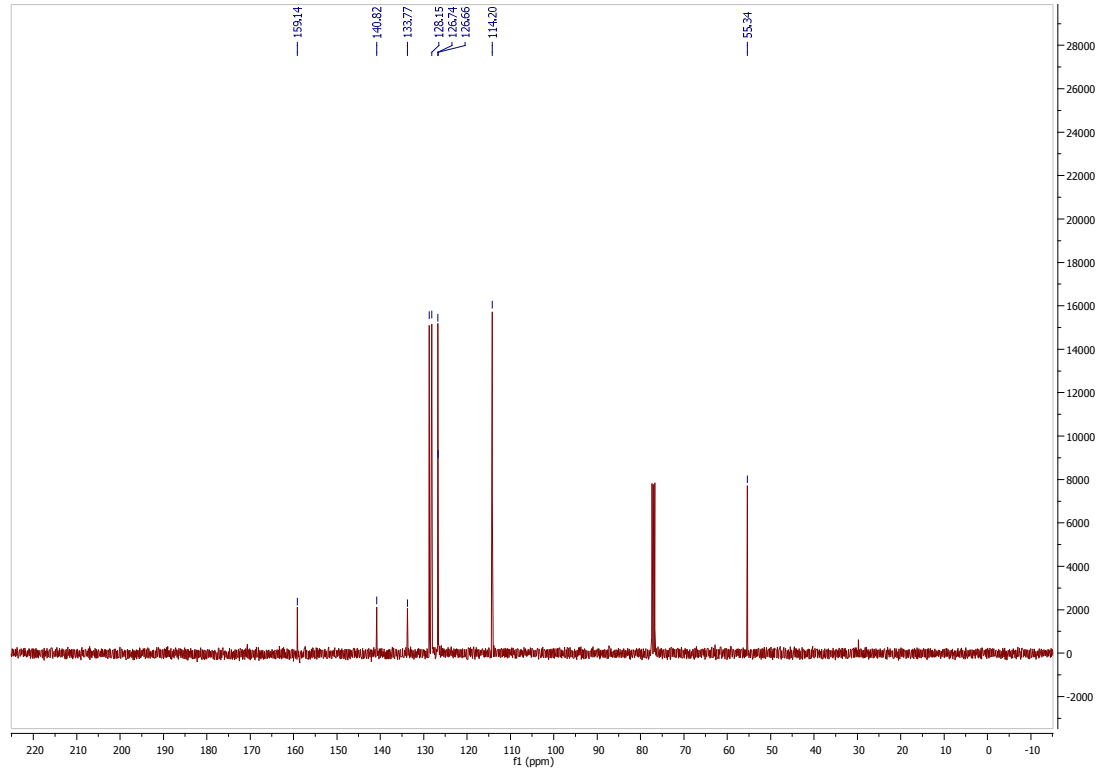
128.75
128.02
127.25
127.16
126.58
126.46
21.06
20.39
f1 (ppm)


7.59
7.57
7.55
7.46
7.44
7.42
7.35
7.33
7.31
7.02
6.99
3.87
MeO
2o
2.03
1.02
0.49
1.00
1.72
f1 (ppm)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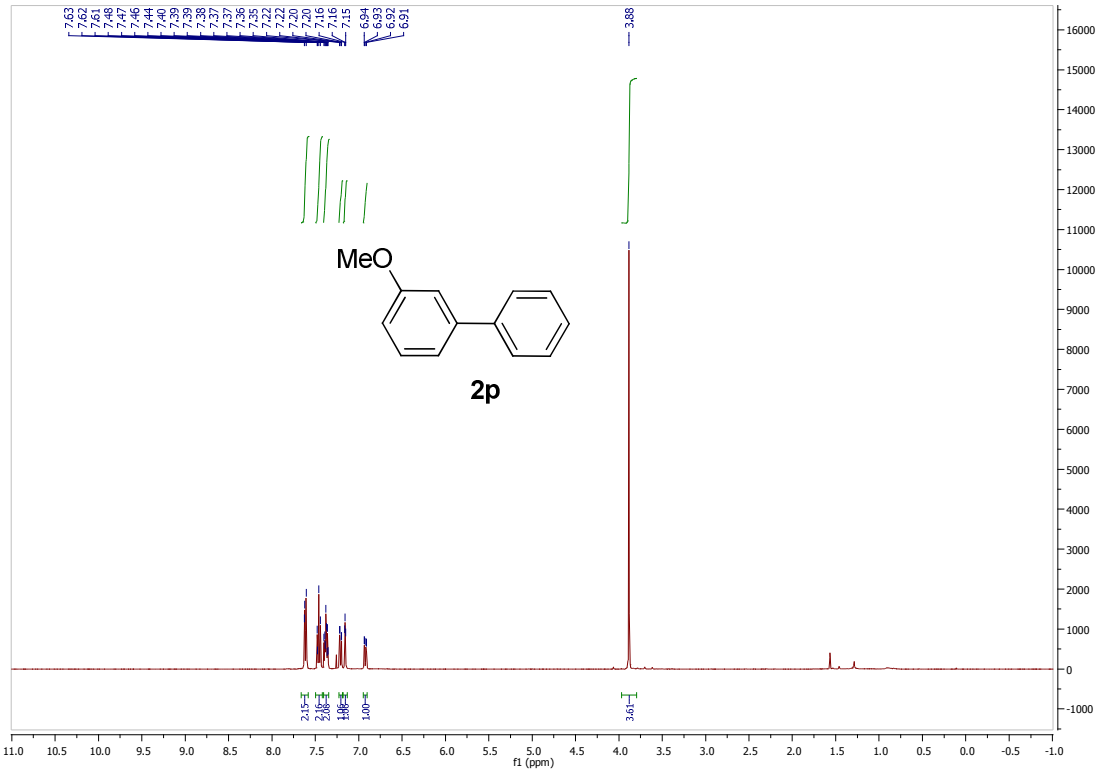
126.74
126.66
114.20
55.34
f1 (ppm)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7.62
7.61
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7.47
7.46
7.44
7.40
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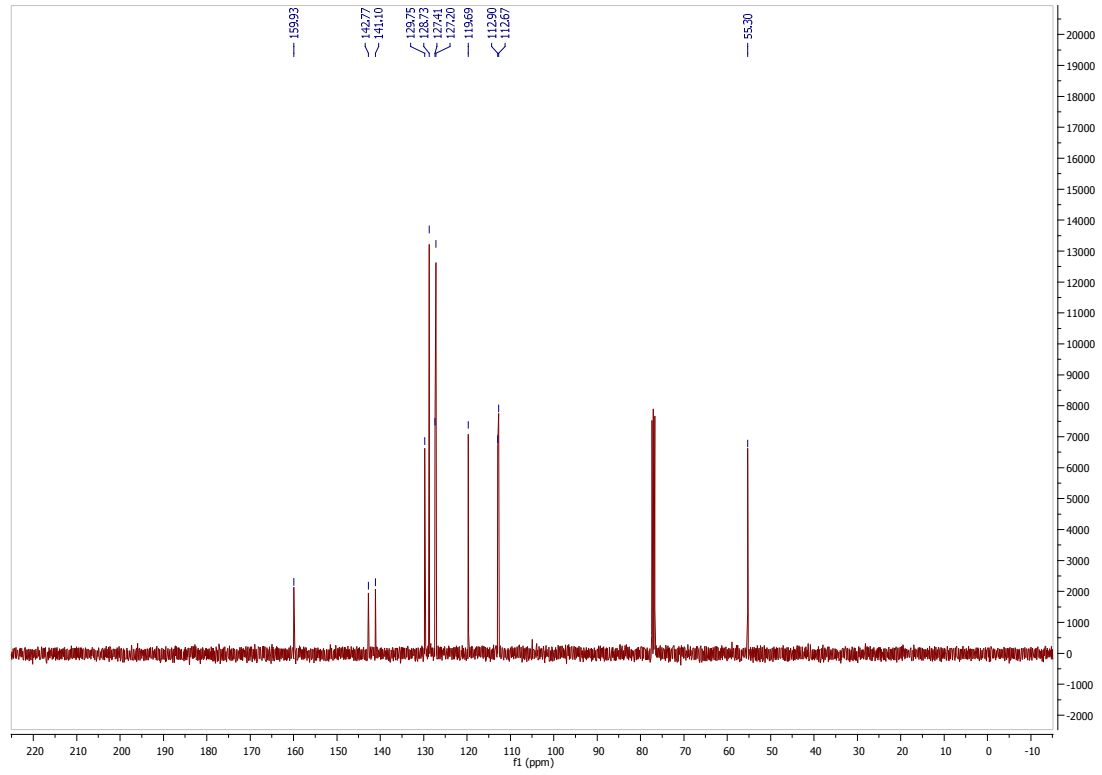
7.39
7.38
7.37
7.36
7.35
7.22
7.22
7.20
7.20
7.16
7.16
7.15
6.94
6.93
6.92
6.91
3.88
MeO
2p
2.15
2.16
2.06
1.00
3.61
f1 (ppm)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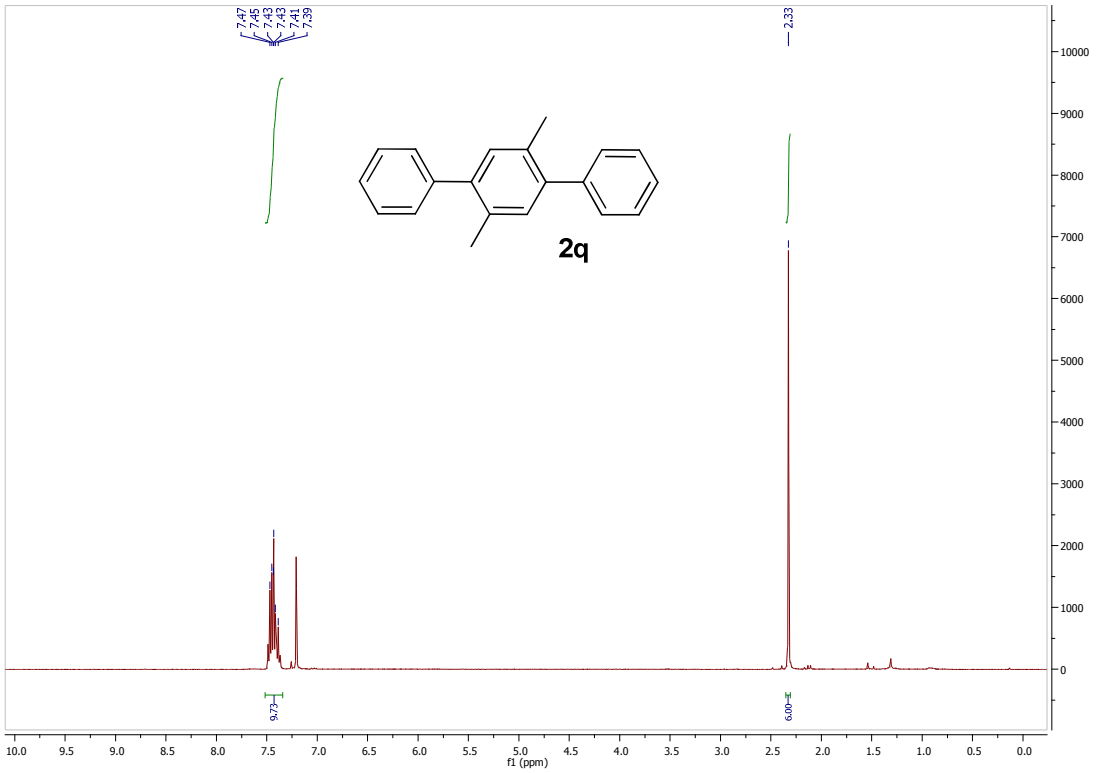
127.41
127.20
119.69
112.90
112.67
55.30
f1 (ppm)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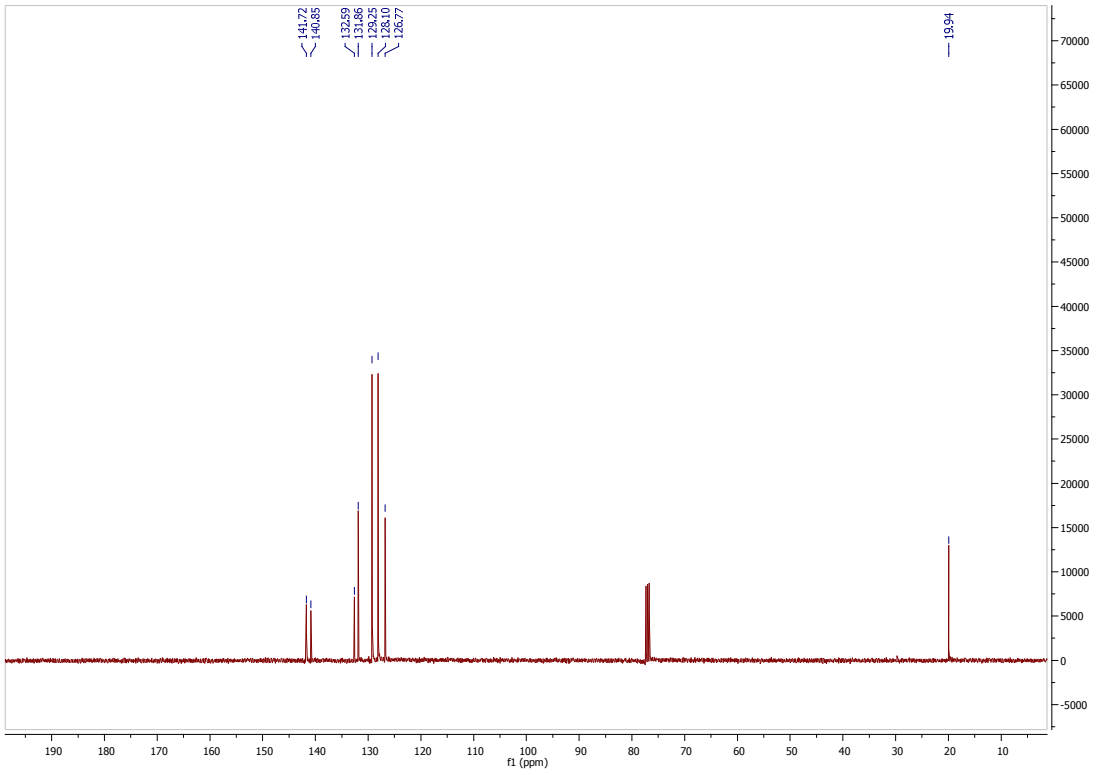
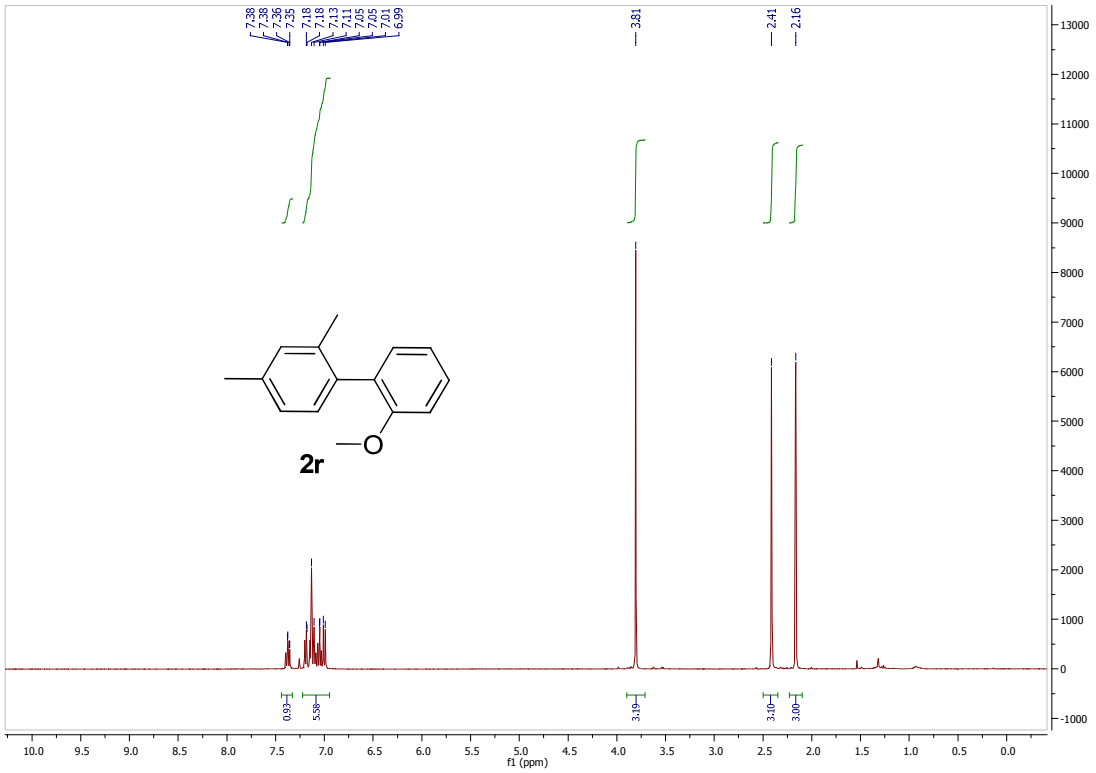
7.43
7.41
7.39
2.33
2q
9.73
6.00
f1 (ppm)


141.72
140.85
132.59
131.86
129.25
128.10
126.77
19.94
f1 (ppm)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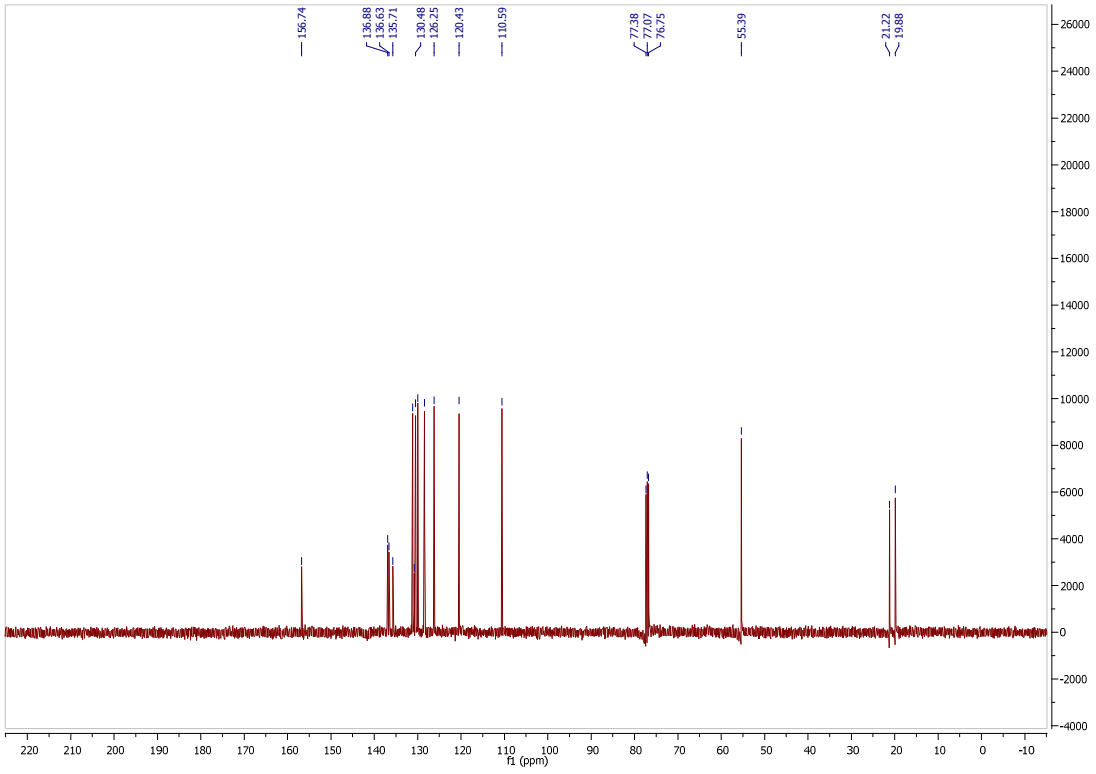
7.38
7.36
7.35
7.18
7.18
7.13
7.11
7.05
7.05
7.01
6.99
3.81
2.41
2.16
O
2r
0.93
5.58
3.19
3.10
3.00
f1 (ppm)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136.88
136.63
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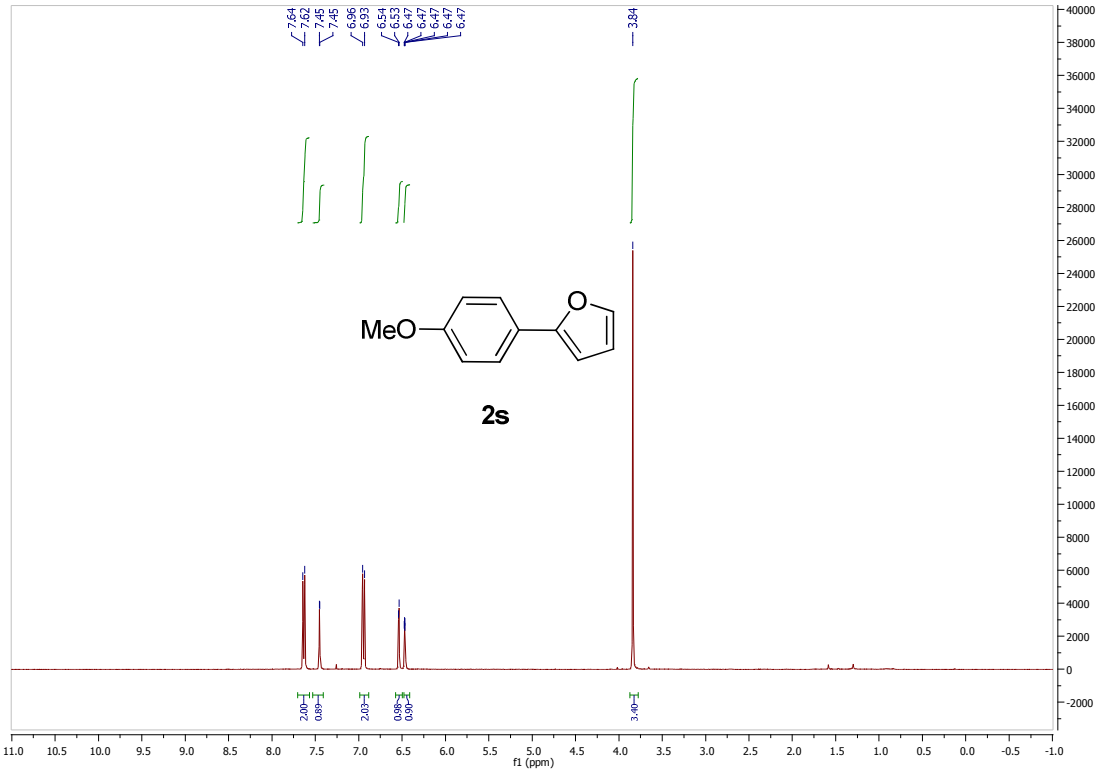
130.48
126.25
120.43
110.59
77.38
77.07
76.75
55.39
21.22
19.88
f1 (ppm)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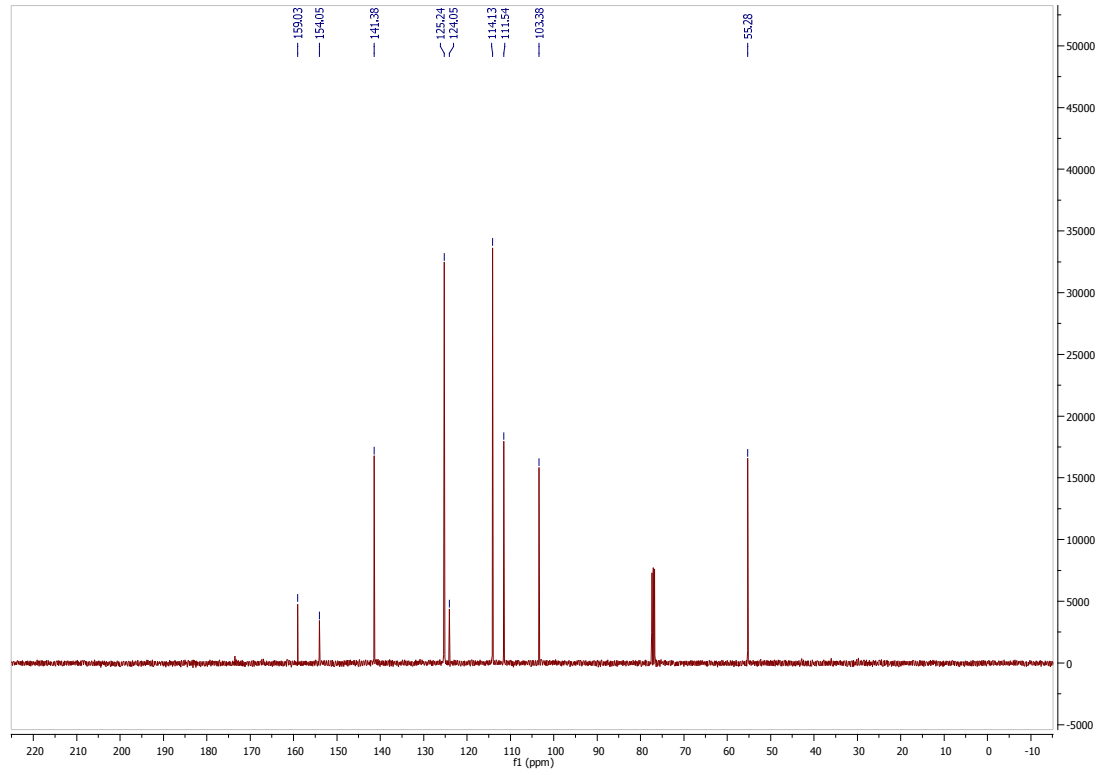
7.62
7.45
7.45
6.96
6.93
6.54
6.53
6.47
6.47
6.47
6.47
6.47
3.84
MeO
O
2s
2.00
0.89
2.03
0.98
0.93
3.40
f1 (ppm)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154.05
141.38
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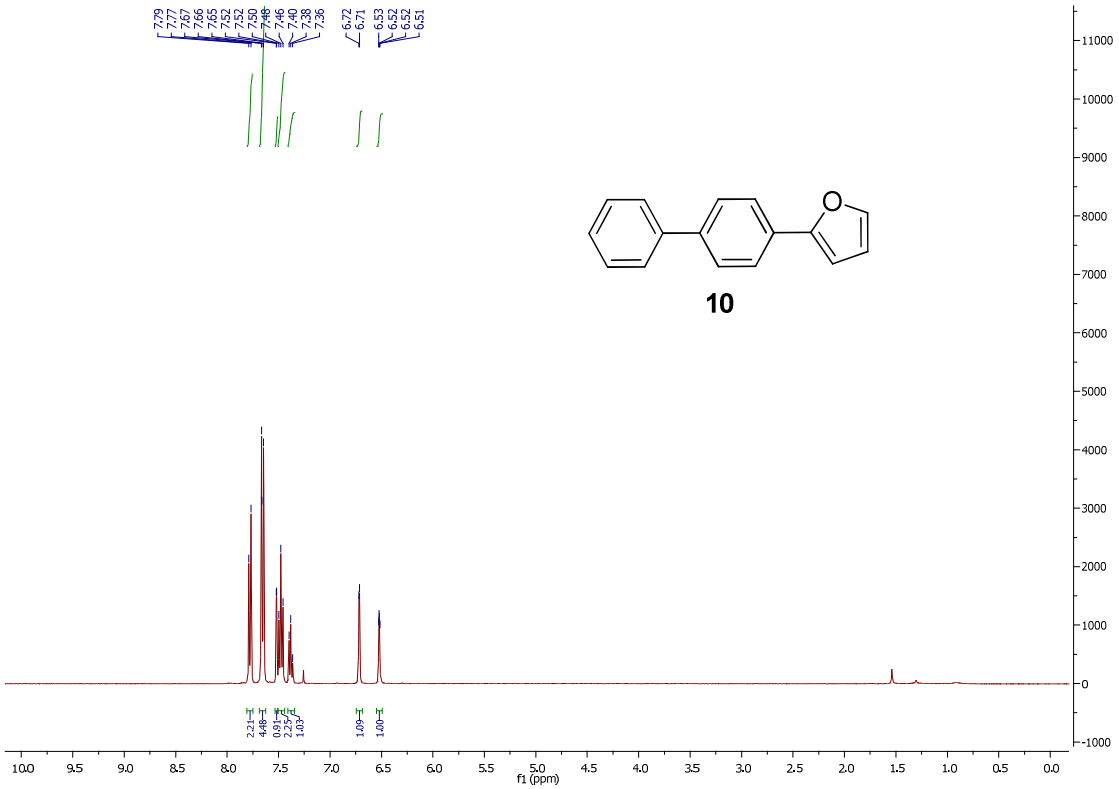
124.05
114.13
111.54
103.38
55.28
f1 (ppm)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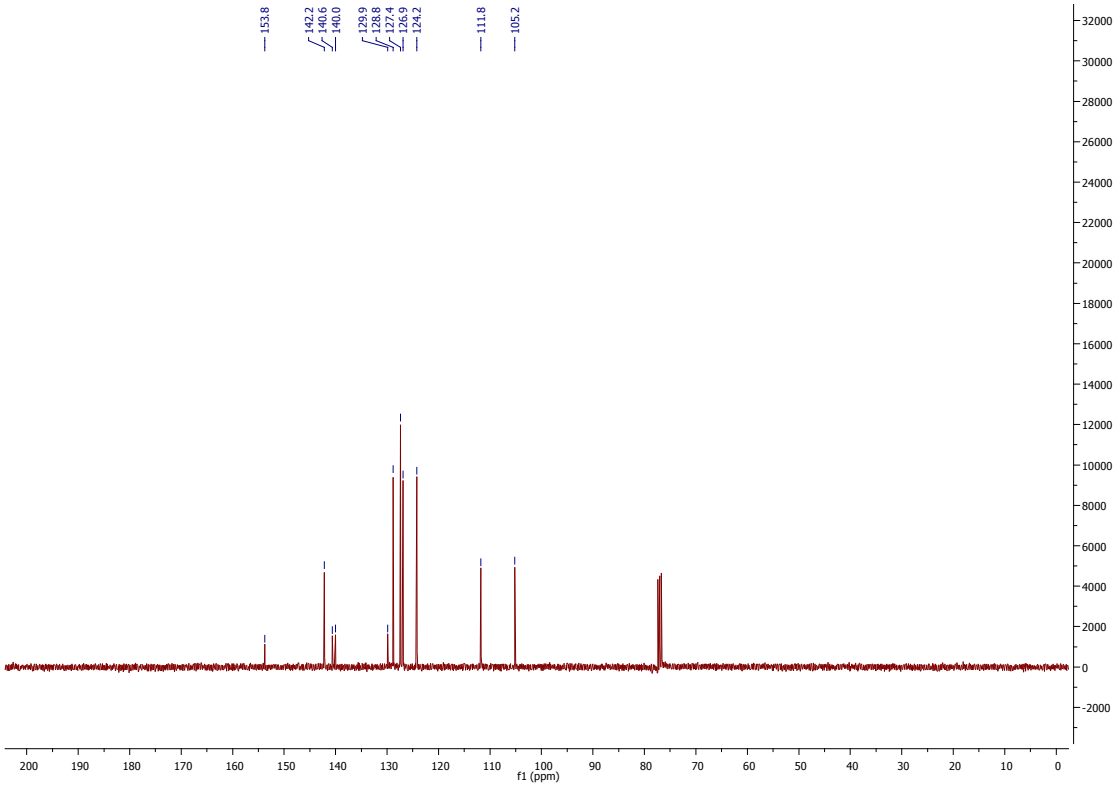
7.65
7.52
7.52
7.50
7.48
7.46
7.40
7.38
7.36
6.72
6.71
6.53
6.52
6.52
6.51
O
10
2.21
4.48
0.91
2.25
1.03
1.09
1.00
f1 (ppm)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140.0
129.9
128.8
127.4
126.9
124.2
111.8
105.2
f1 (ppm)